

10/657,033

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PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * Welcome to STN International * * * * *

NEWS	1		Web Page URLs for STN Seminar Schedule - N. America
NEWS	2		"Ask CAS" for self-help around the clock
NEWS	3	FEB 25	CA/CAPLUS - Russian Agency for Patents and Trademarks (ROSPATENT) added to list of core patent offices covered
NEWS	4	FEB 28	PATDPAFULL - New display fields provide for legal status data from INPADOC
NEWS	5	FEB 28	BABS - Current-awareness alerts (SDIs) available
NEWS	6	FEB 28	MEDLINE/LMEDLINE reloaded
NEWS	7	MAR 02	GBFULL: New full-text patent database on STN
NEWS	8	MAR 03	REGISTRY/ZREGISTRY - Sequence annotations enhanced
NEWS	9	MAR 03	MEDLINE file segment of TOXCENTER reloaded
NEWS	10	MAR 22	KOREAPAT now updated monthly; patent information enhanced
NEWS	11	MAR 22	Original IDE display format returns to REGISTRY/ZREGISTRY
NEWS	12	MAR 22	PATDPASPC - New patent database available
NEWS	13	MAR 22	REGISTRY/ZREGISTRY enhanced with experimental property tags
NEWS	14	APR 04	EPFULL enhanced with additional patent information and new fields
NEWS	15	APR 04	EMBASE - Database reloaded and enhanced
NEWS EXPRESS			JANUARY 10 CURRENT WINDOWS VERSION IS V7.01a, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 10 JANUARY 2005
NEWS HOURS			STN Operating Hours Plus Help Desk Availability
NEWS INTER			General Internet Information
NEWS LOGIN			Welcome Banner and News Items
NEWS PHONE			Direct Dial and Telecommunication Network Access to STN
NEWS WWW			CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that specific topic.

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* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 19:08:48 ON 15 APR 2005

=> file reg

10/657,033

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 19:08:57 ON 15 APR 2005
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STRUCTURE FILE UPDATES: 14 APR 2005 HIGHEST RN 848555-82-8
DICTIONARY FILE UPDATES: 14 APR 2005 HIGHEST RN 848555-82-8

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

*
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
*

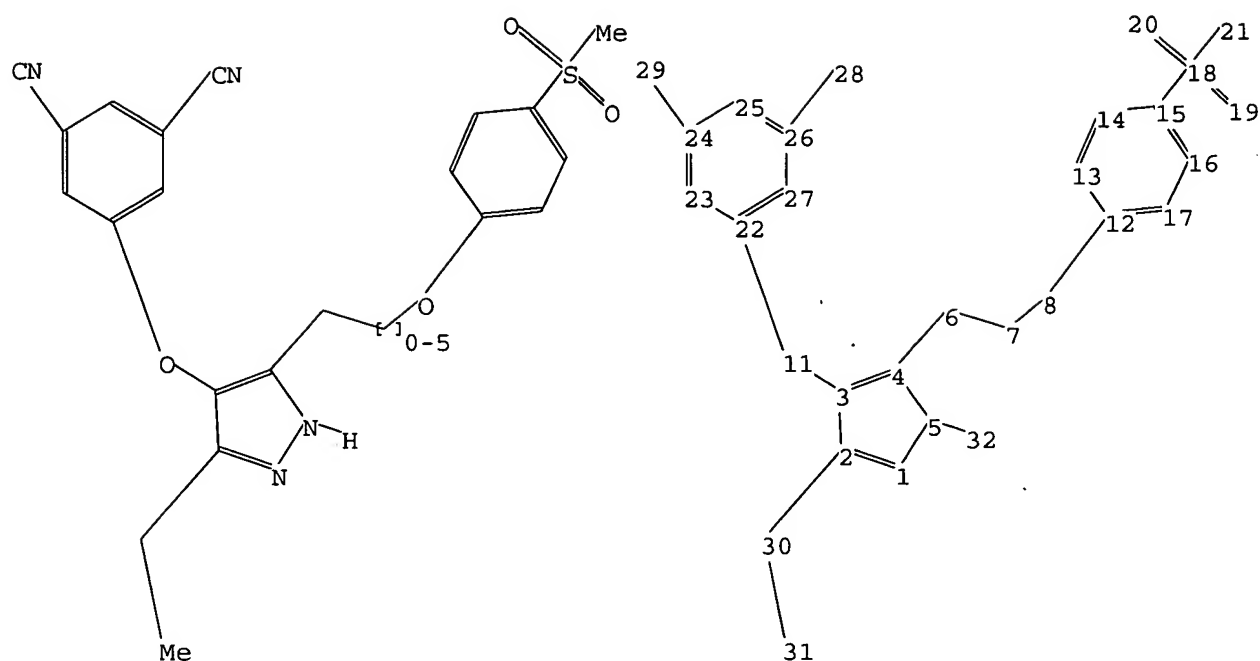
Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10657033.str

10/657,033



```
chain nodes :
6 7 8 11 18 19 20 21 28 29 30 31 32
ring nodes :
1 2 3 4 5 12 13 14 15 16 17 22 23 24 25 26 27
chain bonds :
2-30 3-11 4-6 5-32 6-7 7-8 8-12 11-22 15-18 18-19 18-20 18-21 24-29
26-28 30-31
ring bonds :
1-2 1-5 2-3 3-4 4-5 12-13 12-17 13-14 14-15 15-16 16-17 22-23 22-27
23-24 24-25 25-26 26-27
exact/norm bonds :
1-2 1-5 2-3 3-4 3-11 4-5 7-8 8-12 11-22 15-18 18-19 18-20
exact bonds :
2-30 4-6 5-32 6-7 18-21 24-29 26-28 30-31
normalized bonds :
12-13 12-17 13-14 14-15 15-16 16-17 22-23 22-27 23-24 24-25 25-26 26-27
```

```
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 11:CLASS
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:CLASS 19:CLASS 20:CLASS
21:CLASS 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:CLASS 29:CLASS
30:CLASS 31:CLASS 32:CLASS
```

L1 STRUCTURE UPLOADED

```
=> s l1
SAMPLE SEARCH INITIATED 19:09:20 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 0 TO ITERATE
```

100.0% PROCESSED 0 ITERATIONS 0 ANSWERS

10/657,033

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 0 TO 0
PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s l1 ful
FULL SEARCH INITIATED 19:09:27 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 3 TO ITERATE

100.0% PROCESSED 3 ITERATIONS 1 ANSWERS
SEARCH TIME: 00.00.01

L3 1 SEA SSS FUL L1

=> d l3 ibib hitstr abs
'IBIB' IS NOT A VALID FORMAT FOR FILE 'REGISTRY'
'HITSTR' IS NOT A VALID FORMAT FOR FILE 'REGISTRY'
'ABS' IS NOT A VALID FORMAT FOR FILE 'REGISTRY'

The following are valid formats:

Substance information can be displayed by requesting individual fields or predefined formats. The predefined substance formats are: (RN = CAS Registry Number)

REG - RN
SAM - Index Name, MF, and structure - no RN
FIDE - All substance data, except sequence data
IDE - FIDE, but only 50 names
SQIDE - IDE, plus sequence data
SQIDE3 - Same as SQIDE, but 3-letter amino acid codes are used
SQD - Protein sequence data, includes RN
SQD3 - Same as SQD, but 3-letter amino acid codes are used
SQN - Protein sequence name information, includes RN

CALC - Table of calculated properties
EPROP - Table of experimental properties
PROP - EPROP and CALC

Any CA File format may be combined with any substance format to obtain CA references citing the substance. The substance formats must be cited first. The CA File predefined formats are:

ABS -- Abstract
APPS -- Application and Priority Information
BIB -- CA Accession Number, plus Bibliographic Data
CAN -- CA Accession Number
CBIB -- CA Accession Number, plus Bibliographic Data (compressed)
IND -- Index Data
IPC -- International Patent Classification
PATS -- PI, SO
STD -- BIB, IPC, and NCL

IABS -- ABS, indented, with text labels
IBIB -- BIB, indented, with text labels

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ISTD -- STD format, indented

OBIB ----- AN, plus Bibliographic Data (original)

OIBIB ----- OBIB, indented with text labels

SBIB ----- BIB, no citations

SIBIB ----- IBIB, no citations

The ALL format gives FIDE BIB ABS IND RE, plus sequence data when it is available.

The MAX format is the same as ALL.

The IALL format is the same as ALL with BIB ABS and IND indented, with text labels.

For additional information, please consult the following help messages:

HELP DFIELDS -- To see a complete list of individual display fields.

HELP FORMATS -- To see detailed descriptions of the predefined formats.

ENTER DISPLAY FORMAT (IDE):0

'0' IS NOT A VALID FORMAT FOR FILE 'REGISTRY'

The following are valid formats:

Substance information can be displayed by requesting individual fields or predefined formats. The predefined substance formats are: (RN = CAS Registry Number)

REG - RN

SAM - Index Name, MF, and structure - no RN

FIDE - All substance data, except sequence data

IDE - FIDE, but only 50 names

SQIDE - IDE, plus sequence data

SQIDE3 - Same as SQIDE, but 3-letter amino acid codes are used

SQD - Protein sequence data, includes RN

SQD3 - Same as SQD, but 3-letter amino acid codes are used

SQN - Protein sequence name information, includes RN

CALC - Table of calculated properties

EPROP - Table of experimental properties

PROP - EPROP and CALC

Any CA File format may be combined with any substance format to obtain CA references citing the substance. The substance formats must be cited first. The CA File predefined formats are:

ABS -- Abstract

APPS -- Application and Priority Information

BIB -- CA Accession Number, plus Bibliographic Data

CAN -- CA Accession Number

CBIB -- CA Accession Number, plus Bibliographic Data (compressed)

IND -- Index Data

IPC -- International Patent Classification

PATS -- PI, SO

STD -- BIB, IPC, and NCL

IABS -- ABS, indented, with text labels

IBIB -- BIB, indented, with text labels

ISTD -- STD format, indented

10/657,033

OBIB ----- AN, plus Bibliographic Data (original)
OIBIB ----- OBIB, indented with text labels

SBIB ----- BIB, no citations
SIBIB ----- IBIB, no citations

The ALL format gives FIDE BIB ABS IND RE, plus sequence data when it is available.

The MAX format is the same as ALL.

The IALL format is the same as ALL with BIB ABS and IND indented, with text labels.

For additional information, please consult the following help messages:

HELP DFIELDS -- To see a complete list of individual display fields.
HELP FORMATS -- To see detailed descriptions of the predefined formats.
ENTER DISPLAY FORMAT (IDE):end

=> file caplus
COST IN U.S. DOLLARS

FULL ESTIMATED COST

SINCE FILE	TOTAL
ENTRY	SESSION
161.76	161.97

FILE 'CAPLUS' ENTERED AT 19:09:57 ON 15 APR 2005
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FILE COVERS 1907 - 15 Apr 2005 VOL 142 ISS 17
FILE LAST UPDATED: 14 Apr 2005 (20050414/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l3
L4 1 L3

=> d his

(FILE 'HOME' ENTERED AT 19:08:48 ON 15 APR 2005)

FILE 'REGISTRY' ENTERED AT 19:08:57 ON 15 APR 2005

L1 STRUCTURE UPLOADED
L2 0 S L1
L3 1 S L1 FUL

10/657,033

FILE 'CAPLUS' ENTERED AT 19:09:57 ON 15 APR 2005

L4 1 S L3

=> d l4 ibib hitstr abs

L4 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:308421 CAPLUS

DOCUMENT NUMBER: 140:321351

TITLE: Preparation of pyrazole derivatives as therapeutic agents for HIV mediated diseases

INVENTOR(S): Edwards, Paul John; Jones, Lyn Howard; Mowbray, Charles Eric; Stupple, Paul Anthony; Tran, Isabelle

PATENT ASSIGNEE(S): Pfizer Limited, UK; Pfizer Inc.

SOURCE: PCT Int. Appl., 45 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004031156	A1	20040415	WO 2003-IB4214	20030924
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
US 2005054707	A1	20050310	US 2003-657033	20030905
PRIORITY APPLN. INFO.:			GB 2002-23234	A 20021007

OTHER SOURCE(S): MARPAT 140:321351

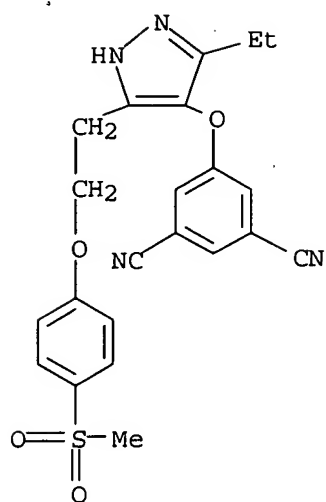
IT 678992-82-0P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

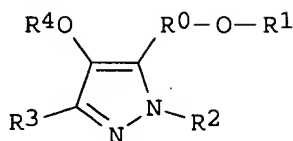
(preparation of pyrazole derivs. as therapeutic agents for HIV mediated diseases)

RN 678992-82-0 CAPLUS

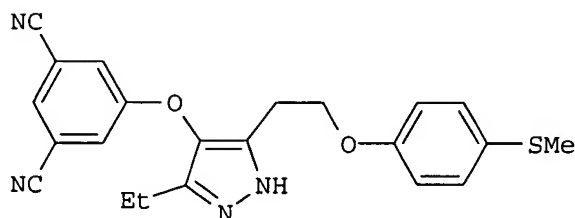
CN 1,3-Benzenedicarbonitrile, 5-[[[3-ethyl-5-[2-[4-(methylsulfonyl)phenoxy]ethyl]-1H-pyrazol-4-yl]oxy]- (9CI) (CA INDEX NAME)



GI



I



II

AB The title compds. [I; R⁰ = absent, alkylene; R¹ = Ph substituted by SO_yR₅, alkylene(SO_yR₅), SO_yCF₃, etc.; R₂ = H, alkyl, cycloalkyl, etc.; R₃ = H, alkyl, cycloalkyl, Ph, etc.; R₄ = (un)substituted Ph, naphthyl, pyridyl; R₅ = H, alkyl, cycloalkyl, etc.; y = 0-2] which bind to the enzyme reverse transcriptase and are modulators, especially inhibitors thereof, and as such are

useful in the treatment of a variety of disorders including those in which the inhibition of reverse transcriptase is implicated, were prepared and formulated. Disorders of interest include those caused by Human Immunodeficiency Virus (HIV) and genetically related retroviruses, such as Acquired Immune Deficiency Syndrome (AIDS). Thus, reacting 5-{[3-ethyl-5-(2-hydroxyethyl)-1H-pyrazol-4-yl]oxy}isophthalonitrile (preparation given) with 4-(methylmercapto)phenol afforded I [R⁰ = (CH₂)₂; R¹ = 4-(MeS)C₆H₄; R₂ = H; R₃ = Et; R₄ = 3,5-(NC)₂C₆H₃] which showed IC₅₀ of 2 nM against HIV-1 reverse transcriptase. The pharmaceutical composition comprising the compound I is claimed.

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS

10/657,033

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> file reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

6.29

168.26

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

-0.73

-0.73

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STRUCTURE FILE UPDATES: 14 APR 2005 HIGHEST RN 848555-82-8

DICTIONARY FILE UPDATES: 14 APR 2005 HIGHEST RN 848555-82-8

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

Please note that search-term pricing does apply when conducting SmartSELECT searches.

*
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
*

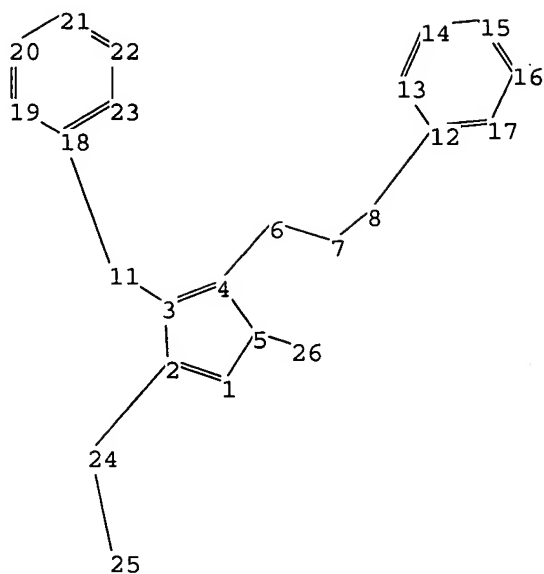
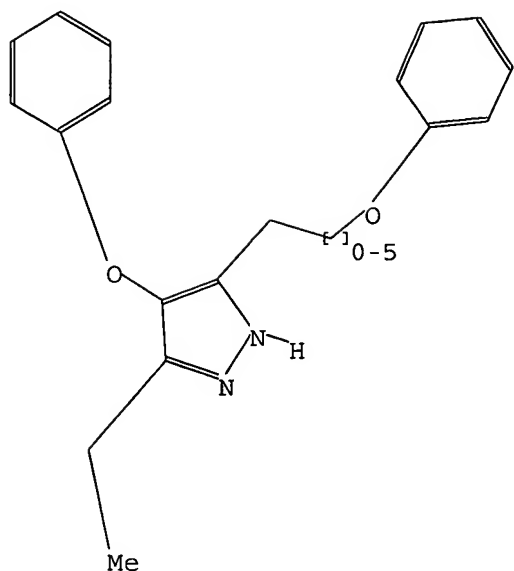
Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>

Uploading C:\Program Files\Stnexp\Queries\106570331.str

10/657,033



chain nodes :

6 7 8 11 24 25 26

ring nodes :

1 2 3 4 5 12 13 14 15 16 17 18 19 20 21 22 23

chain bonds :

2-24 3-11 4-6 5-26 6-7 7-8 8-12 11-18 24-25

ring bonds :

1-2 1-5 2-3 3-4 4-5 12-13 12-17 13-14 14-15 15-16 16-17 18-19 18-23
19-20 20-21 21-22 22-23

exact/norm bonds :

1-2 1-5 2-3 3-4 3-11 4-5 7-8 8-12 11-18

exact bonds :

2-24 4-6 5-26 6-7 24-25

normalized bonds :

12-13 12-17 13-14 14-15 15-16 16-17 18-19 18-23 19-20 20-21 21-22 22-23

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 11:CLASS
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom
21:Atom 22:Atom 23:Atom 24:CLASS 25:CLASS 26:CLASS

L5 STRUCTURE UPLOADED

=> s 15

SAMPLE SEARCH INITIATED 19:11:48 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 1 TO ITERATE

100.0% PROCESSED 1 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 1 TO 80

10/657,033

PROJECTED ANSWERS: 0 TO 0

L6 0 SEA SSS SAM L5

=> s 15 ful
FULL SEARCH INITIATED 19:11:57 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 21 TO ITERATE

100.0% PROCESSED 21 ITERATIONS 7 ANSWERS
SEARCH TIME: 00.00.01

L7 7 SEA SSS FUL L5

	SINCE FILE ENTRY	TOTAL SESSION
=> file caplus		
COST IN U.S. DOLLARS		
FULL ESTIMATED COST	161.33	329.59
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)		
CA SUBSCRIBER PRICE	0.00	-0.73

FILE 'CAPLUS' ENTERED AT 19:12:03 ON 15 APR 2005
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FILE COVERS 1907 - 15 Apr 2005 VOL 142 ISS 17
FILE LAST UPDATED: 14 Apr 2005 (20050414/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 16
L8 0 L6

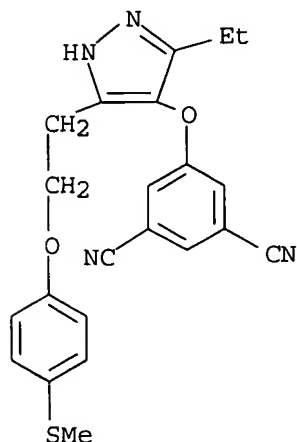
=> s 17
L9 2 L7

=> d 19 ibib hitstr abs

L9 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:308421 CAPLUS
DOCUMENT NUMBER: 140:321351
TITLE: Preparation of pyrazole derivatives as therapeutic agents for HIV mediated diseases
INVENTOR(S): Edwards, Paul John; Jones, Lyn Howard; Mowbray,

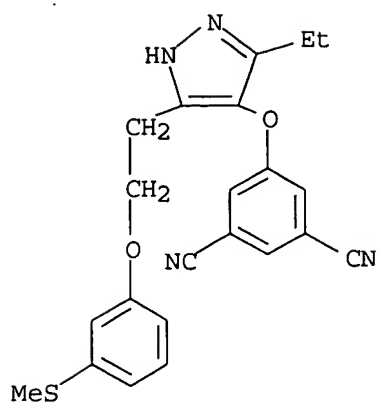
PATENT ASSIGNEE(S): Charles Eric; Stupple, Paul Anthony; Tran, Isabelle
 SOURCE: Pfizer Limited, UK; Pfizer Inc.
 PCT Int. Appl., 45 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004031156	A1	20040415	WO 2003-IB4214	20030924
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2005054707	A1	20050310	US 2003-657033	20030905
PRIORITY APPLN. INFO.:			GB 2002-23234	A 20021007
OTHER SOURCE(S):		MARPAT 140:321351		
IT 678992-80-8P 678992-83-1P 678992-84-2P				
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses) (preparation of pyrazole derivs. as therapeutic agents for HIV mediated diseases)				
RN	678992-80-8 CAPLUS			
CN	1,3-Benzenedicarbonitrile, 5-[[3-ethyl-5-[2-[4-(methylthio)phenoxy]ethyl]-1H-pyrazol-4-yl]oxy]- (9CI) (CA INDEX NAME)			



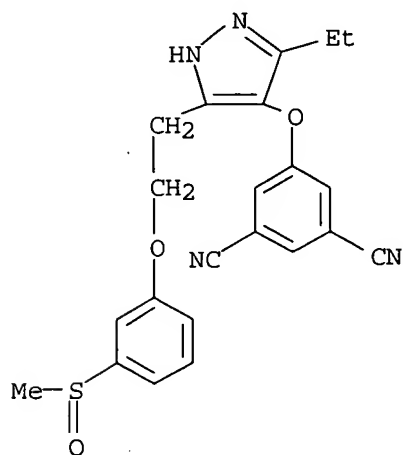
RN 678992-83-1 CAPLUS
 CN 1,3-Benzenedicarbonitrile, 5-[[3-ethyl-5-[2-[3-(methylthio)phenoxy]ethyl]-1H-pyrazol-4-yl]oxy]- (9CI) (CA INDEX NAME)

10/657,033



RN 678992-84-2 CAPLUS

CN 1,3-Benzenedicarbonitrile, 5-[[3-ethyl-5-[2-[3-(methylsulfinyl)phenoxy]ethyl]-1H-pyrazol-4-yl]oxy]- (9CI) (CA INDEX NAME)



IT 678992-81-9P 678992-82-0P 678992-85-3P

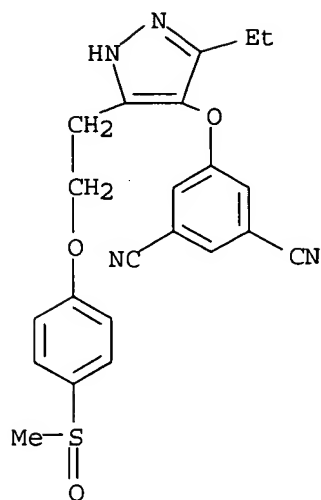
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of pyrazole derivs. as therapeutic agents for HIV mediated diseases)

RN 678992-81-9 CAPLUS

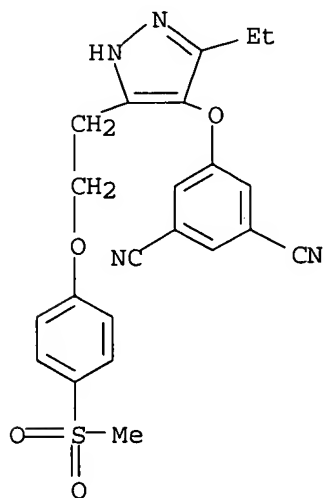
CN 1,3-Benzenedicarbonitrile, 5-[[3-ethyl-5-[2-[4-(methylsulfonyl)phenoxy]ethyl]-1H-pyrazol-4-yl]oxy]- (9CI) (CA INDEX NAME)

10/657,033



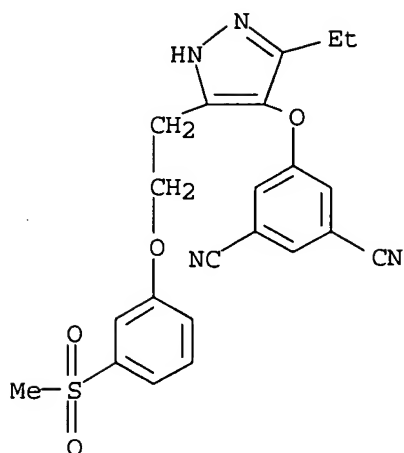
RN 678992-82-0 CAPLUS

CN 1,3-Benzenedicarbonitrile, 5-[[3-ethyl-5-[2-[4-(methylsulfonyl)phenoxy]ethyl]-1H-pyrazol-4-yl]oxy] - (9CI) (CA INDEX NAME)

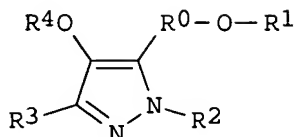


RN 678992-85-3 CAPLUS

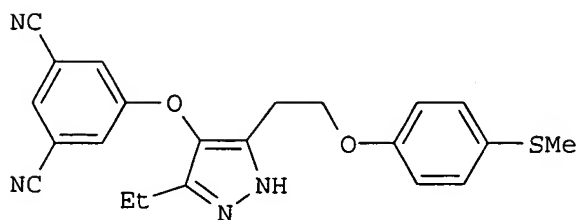
CN 1,3-Benzenedicarbonitrile, 5-[[3-ethyl-5-[2-[3-(methylsulfonyl)phenoxy]ethyl]-1H-pyrazol-4-yl]oxy] - (9CI) (CA INDEX NAME)



GI



I



II

AB The title compds. [I; R0 = absent, alkylene; R1 = Ph substituted by SOyR5, alkylene(SOyR5), SOyCF3, etc.; R2 = H, alkyl, cycloalkyl, etc.; R3 = H, alkyl, cycloalkyl, Ph, etc.; R4 = (un)substituted Ph, naphthyl, pyridyl; R5 = H, alkyl, cycloalkyl, etc.; y = 0-2] which bind to the enzyme reverse transcriptase and are modulators, especially inhibitors thereof, and as such are

useful in the treatment of a variety of disorders including those in which the inhibition of reverse transcriptase is implicated, were prepared and formulated. Disorders of interest include those caused by Human Immunodeficiency Virus (HIV) and genetically related retroviruses, such as Acquired Immune Deficiency Syndrome (AIDS). Thus, reacting 5-([3-ethyl-5-(2-hydroxyethyl)-1H-pyrazol-4-yl]oxy)isophthalonitrile (preparation given) with 4-(methylmercapto)phenol afforded I [R0 = (CH2)2; R1 = 4-(MeS)C6H4; R2 = H; R3 = Et; R4 = 3,5-(NC)2C6H3] which showed IC50 of 2 nM against HIV-1 reverse transcriptase. The pharmaceutical composition comprising the compound I is claimed.

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d 19 ibib hitstr abs 2

L9 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 2002:832763 CAPLUS
 DOCUMENT NUMBER: 137:337884
 TITLE: Preparation of aryloxy pyrazole derivatives as reverse transcriptase inhibitors for treating HIV
 INVENTOR(S): Jones, Lyn Howard; Mowbray, Charles Eric; Price, Davis Anthony; Selby, Matthew Duncan; Stupple, Paul Anthony
 PATENT ASSIGNEE(S): Pfizer Limited, UK; Pfizer Inc.
 SOURCE: PCT Int. Appl., 306 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
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EP 1377556	A1	20040107	EP 2002-708600	20020404
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BR 2002008811	A	20040309	BR 2002-8811	20020404
JP 2004531535	T2	20041014	JP 2002-583387	20020404
US 2003100554	A1	20030529	US 2002-118512	20020405
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OTHER SOURCE(S): MARPAT 137:337884

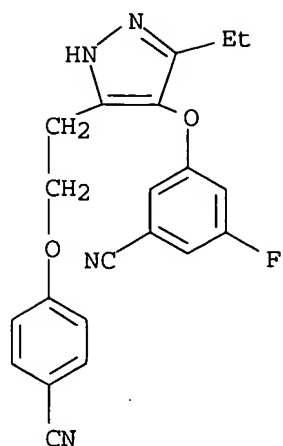
IT 473921-42-5P, 3-[[5-[2-(4-Cyanophenoxy)ethyl]-3-ethyl-1H-pyrazol-4-yl]oxy]-5-fluorobenzonitrile

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

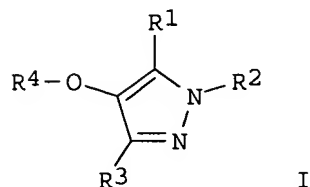
(drug candidate; preparation of aryloxy pyrazole derivs. as reverse transcriptase inhibitors for treating HIV)

RN 473921-42-5 CAPLUS

CN Benzonitrile, 3-[[5-[2-(4-cyanophenoxy)ethyl]-3-ethyl-1H-pyrazol-4-yl]oxy]-5-fluoro- (9CI) (CA INDEX NAME)



GI



I

AB This invention relates to pyrazole derivs. (shown as I; e.g. 2-Amino-6-[[4-(3,5-dichlorophenoxy)-3,5-diethyl-1H-pyrazol-1-yl]methyl]-4(3H)-pyrimidinone) or pharmaceutically acceptable salts, solvates or derivative thereof, wherein R1 to R4 are defined below, and to processes for the preparation thereof, intermediates used in their preparation of, compns. containing

them and the uses of such derivs. The compds. of the present invention bind to the enzyme reverse transcriptase and are modulators, especially inhibitors thereof. As such the compds. of the present invention are useful in the treatment of a variety of disorders including those in which the inhibition of reverse transcriptase is implicated. Disorders of interest include those caused by Human Immunodeficiency Virus (HIV) and genetically related retroviruses, such as Acquired Immune Deficiency Syndrome (AIDS). In tests of inhibition of HIV-1 reverse transcriptase enzyme, the claimed compds. 2-amino-6-[[4-(3,5-dichlorophenoxy)-3,5-diethyl-1H-pyrazol-1-yl]methyl]-4(3H)-pyrimidinone, 3,5-dimethyl-4-[[3,5-diethyl-1-(2-hydroxyethyl)-1H-pyrazol-4-yl]oxy]benzonitrile and 1-(3-azetidynyl)-4-(3,5-dichlorophenoxy)-3,5-diethyl-1H-pyrazole had IC50 values of 39,000, 3,200 and 248 nM, resp. In I: R1 is H, C1-C6 alkyl, C3-C7 cycloalkyl, Ph, benzyl, halo, -CN, -OR7, -CO2R10, -CONR5R10, R8 or R9. R2 is H, C1-C6 alkyl, C3-C6 alkenyl, C3-C6 alkynyl, C3-C7 cycloalkyl, C3-C7 cycloalkenyl, Ph, benzyl, R8 or R9; or, R1 and R2, when taken together, represent unbranched C3-C4 alkylene. R3 is H, C1-C6 alkyl, C3-C7 cycloalkyl, Ph, benzyl, halo, -CN, -OR7, -CO2R5, -CONR5R5, R8 or R9; R4 is Ph, naphthyl or pyridyl. Definitions of R5 and R7-R10 and addnl. specifications are given in the claims. Included are 283 claimed-compound

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prepns. and 115 intermediate prepns.

REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	12.58	342.17
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-1.46	-2.19

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STRUCTURE FILE UPDATES: 14 APR 2005 HIGHEST RN 848555-82-8
DICTIONARY FILE UPDATES: 14 APR 2005 HIGHEST RN 848555-82-8

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

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*
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
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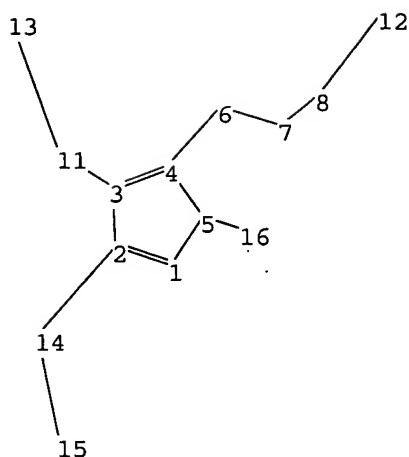
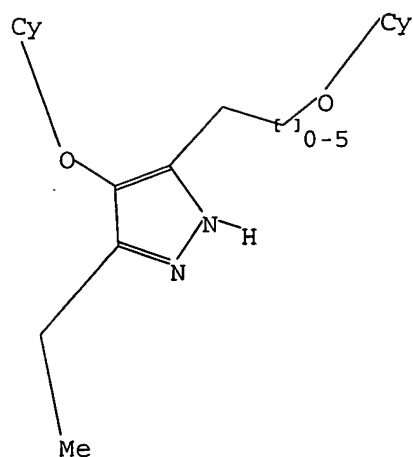
Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
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<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>

Uploading C:\Program Files\Stnexp\Queries\106570332.str

10/657,033



chain nodes :
6 7 8 11 12 13 14 15 16
ring nodes :
1 2 3 4 5
chain bonds :
2-14 3-11 4-6 5-16 6-7 7-8 8-12 11-13 14-15
ring bonds :
1-2 1-5 2-3 3-4 4-5
exact/norm bonds :
1-2 1-5 2-3 3-4 3-11 4-5 7-8 8-12 11-13
exact bonds :
2-14 4-6 5-16 6-7 14-15

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 11:CLASS
12:Atom 13:Atom 14:CLASS 15:CLASS 16:CLASS

L10 STRUCTURE UPLOADED

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SAMPLE SCREEN SEARCH COMPLETED - 24 TO ITERATE

100.0% PROCESSED 24 ITERATIONS 0 ANSWERS
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FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 187 TO 773
PROJECTED ANSWERS: 0 TO 0

L11 0 SEA SSS SAM L10

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FULL SCREEN SEARCH COMPLETED - 645 TO ITERATE

10/657,033

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10 ANSWERS

L12 10 SEA SSS FUL L10

=> file caplus

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DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
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CA SUBSCRIBER PRICE	0.00	-2.19

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FILE COVERS 1907 - 15 Apr 2005 VOL 142 ISS 17
FILE LAST UPDATED: 14 Apr 2005 (20050414/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l12

L13 2 L12

=> file caplus

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	ENTRY	SESSION
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CA SUBSCRIBER PRICE	0.00	-2.19

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FILE LAST UPDATED: 14 Apr 2005 (20050414/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

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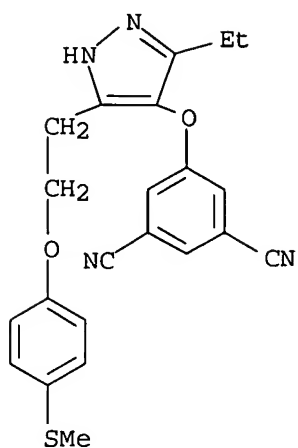
L14 2 L12

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L14 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:308421 CAPLUS
DOCUMENT NUMBER: 140:321351
TITLE: Preparation of pyrazole derivatives as therapeutic agents for HIV mediated diseases
INVENTOR(S): Edwards, Paul John; Jones, Lyn Howard; Mowbray, Charles Eric; Stuppel, Paul Anthony; Tran, Isabelle
PATENT ASSIGNEE(S): Pfizer Limited, UK; Pfizer Inc.
SOURCE: PCT Int. Appl., 45 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

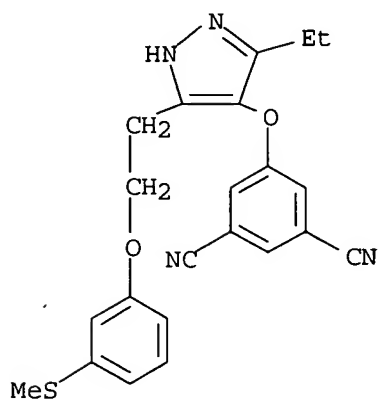
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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2005054707	A1	20050310	US 2003-657033	20030905
PRIORITY APPLN. INFO.:			GB 2002-23234	A 20021007
OTHER SOURCE(S):		MARPAT 140:321351		
IT 678992-80-8P 678992-83-1P 678992-84-2P				
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)				
(preparation of pyrazole derivs. as therapeutic agents for HIV mediated diseases)				
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CN	1,3-Benzenedicarbonitrile, 5-[[3-ethyl-5-[2-[4-(methylthio)phenoxy]ethyl]-1H-pyrazol-4-yl]oxy]- (9CI) (CA INDEX NAME)			

10/657,033



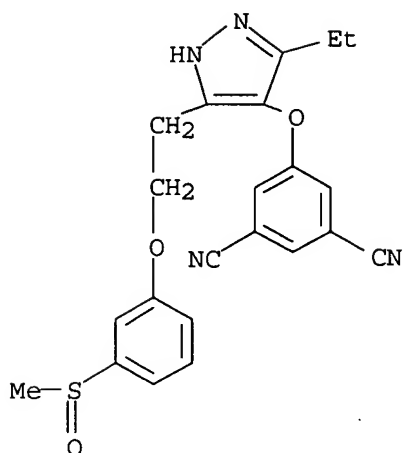
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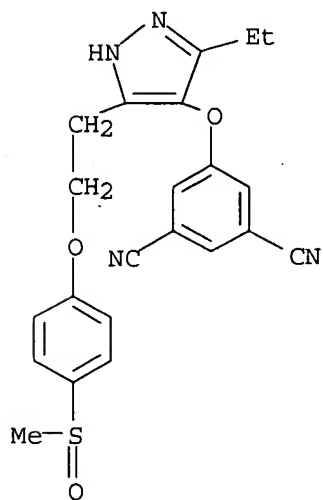


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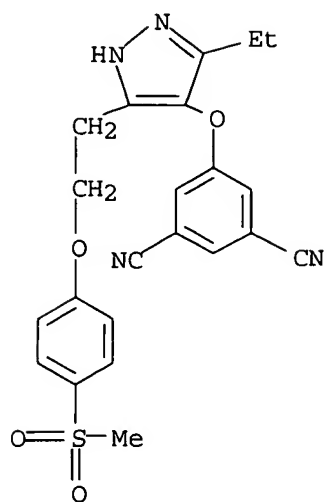


IT 678992-81-9P 678992-82-0P 678992-85-3P
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 (preparation of pyrazole derivs. as therapeutic agents for HIV mediated
 diseases)
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 NAME)



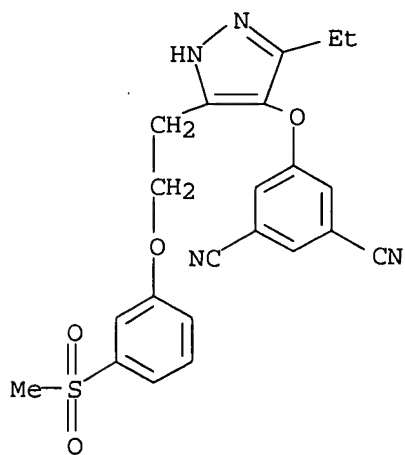
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 NAME)

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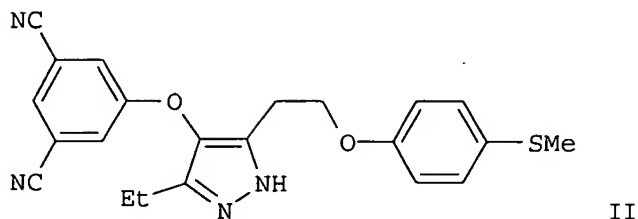
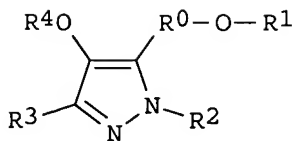


RN 678992-85-3 CAPLUS

CN 1,3-Benzenedicarbonitrile, 5-[[[3-ethyl-5-[2-[3-(methylsulfonyl)phenoxy]ethyl]-1H-pyrazol-4-yl]oxy]- (9CI) (CA INDEX NAME)



GI



AB The title compds. [I; R0 = absent, alkylene; R1 = Ph substituted by SOyR5, alkylene(SOyR5), SOyCF3, etc.; R2 = H, alkyl, cycloalkyl, etc.; R3 = H, alkyl, cycloalkyl, Ph, etc.; R4 = (un)substituted Ph, naphthyl, pyridyl; R5 = H, alkyl, cycloalkyl, etc.; y = 0-2] which bind to the enzyme reverse transcriptase and are modulators, especially inhibitors thereof, and as such are

useful in the treatment of a variety of disorders including those in which the inhibition of reverse transcriptase is implicated, were prepared and formulated. Disorders of interest include those caused by Human Immunodeficiency Virus (HIV) and genetically related retroviruses, such as Acquired Immune Deficiency Syndrome (AIDS). Thus, reacting 5-{[3-ethyl-5-(2-hydroxyethyl)-1H-pyrazol-4-yl]oxy}isophthalonitrile (preparation given) with 4-(methylmercapto)phenol afforded I [R0 = (CH2)2; R1 = 4-(MeS)C6H4; R2 = H; R3 = Et; R4 = 3,5-(NC)2C6H3] which showed IC50 of 2 nM against HIV-1 reverse transcriptase. The pharmaceutical composition comprising the compound I is claimed.

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L14 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2002:832763 CAPLUS

DOCUMENT NUMBER: 137:337884

TITLE: Preparation of aryloxy pyrazole derivatives as reverse transcriptase inhibitors for treating HIV

INVENTOR(S): Jones, Lyn Howard; Mowbray, Charles Eric; Price, Davis Anthony; Selby, Matthew Duncan; Stupple, Paul Anthony

PATENT ASSIGNEE(S): Pfizer Limited, UK; Pfizer Inc.

SOURCE: PCT Int. Appl., 306 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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 GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
 LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
 PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ,
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 TJ, TM
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 EP 1377556 A1 20040107 EP 2002-708600 20020404
 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
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 JP 2004531535 T2 20041014 JP 2002-583387 20020404
 US 2003100554 A1 20030529 US 2002-118512 20020405
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 NO 2003004523 A 20031209 NO 2003-4523 20031009
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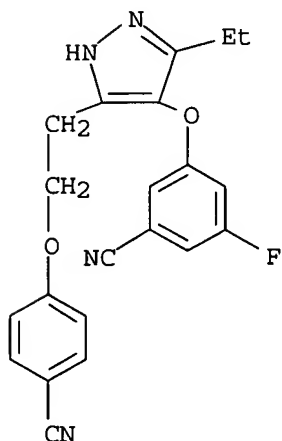
OTHER SOURCE(S): MARPAT 137:337884

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 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of aryloxy pyrazole derivs. as reverse transcriptase inhibitors for treating HIV)

RN 473921-42-5 CAPLUS

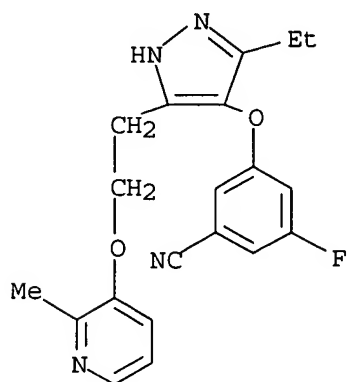
CN Benzonitrile, 3-[[5-[2-(4-cyanophenoxy)ethyl]-3-ethyl-1H-pyrazol-4-yl]oxy]-5-fluoro- (9CI) (CA INDEX NAME)



RN 473921-43-6 CAPLUS

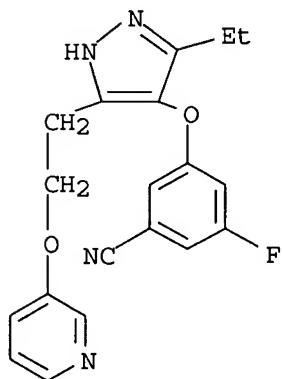
10/657,033

CN Benzonitrile, 3-[[3-ethyl-5-[2-[(2-methyl-3-pyridinyl)oxy]ethyl]-1H-pyrazol-4-yl]oxy]-5-fluoro- (9CI) (CA INDEX NAME)



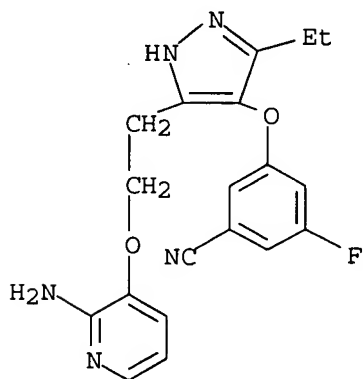
RN 473921-44-7 CAPLUS

CN Benzonitrile, 3-[[3-ethyl-5-[2-(3-pyridinyloxy)ethyl]-1H-pyrazol-4-yl]oxy]-5-fluoro- (9CI) (CA INDEX NAME)

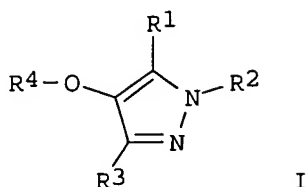


RN 473921-45-8 CAPLUS

CN Benzonitrile, 3-[[5-[2-[(2-amino-3-pyridinyl)oxy]ethyl]-3-ethyl-1H-pyrazol-4-yl]oxy]-5-fluoro- (9CI) (CA INDEX NAME)



GI



AB This invention relates to pyrazole derivs. (shown as I; e.g. 2-Amino-6-[[4-(3,5-dichlorophenoxy)-3,5-diethyl-1H-pyrazol-1-yl]methyl]-4(3H)-pyrimidinone) or pharmaceutically acceptable salts, solvates or derivative thereof, wherein R1 to R4 are defined below, and to processes for the preparation thereof, intermediates used in their preparation of, compns. containing

them and the uses of such derivs. The compds. of the present invention bind to the enzyme reverse transcriptase and are modulators, especially inhibitors thereof. As such the compds. of the present invention are useful in the treatment of a variety of disorders including those in which the inhibition of reverse transcriptase is implicated. Disorders of interest include those caused by Human Immunodeficiency Virus (HIV) and genetically related retroviruses, such as Acquired Immune Deficiency Syndrome (AIDS). In tests of inhibition of HIV-1 reverse transcriptase enzyme, the claimed compds. 2-amino-6-[[4-(3,5-dichlorophenoxy)-3,5-diethyl-1H-pyrazol-1-yl]methyl]-4(3H)-pyrimidinone, 3,5-dimethyl-4-[[3,5-diethyl-1-(2-hydroxyethyl)-1H-pyrazol-4-yl]oxy]benzonitrile and 1-(3-azetidiny)-4-(3,5-dichlorophenoxy)-3,5-diethyl-1H-pyrazole had IC50 values of 39,000, 3,200 and 248 nM, resp. In I: R1 is H, C1-C6 alkyl, C3-C7 cycloalkyl, Ph, benzyl, halo, -CN, -OR7, -CO2R10, -CONR5R10, R8 or R9. R2 is H, C1-C6 alkyl, C3-C6 alkenyl, C3-C6 alkynyl, C3-C7 cycloalkyl, C3-C7 cycloalkenyl, Ph, benzyl, R8 or R9; or, R1 and R2, when taken together, represent unbranched C3-C4 alkylene. R3 is H, C1-C6 alkyl, C3-C7 cycloalkyl, Ph, benzyl, halo, -CN, -OR7, -CO2R5, -CONR5R5, R8 or R9; R4 is Ph, naphthyl or pyridyl. Definitions of R5 and R7-R10 and addnl. specifications are given in the claims. Included are 283 claimed-compound prepsns. and 115 intermediate prepsns.

REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> file reg

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
12.58	516.53

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
-1.46	-3.65

CA SUBSCRIBER PRICE

FILE 'REGISTRY' ENTERED AT 19:19:48 ON 15 APR 2005

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10/657,033

provided by InfoChem.

STRUCTURE FILE UPDATES: 14 APR 2005 HIGHEST RN 848555-82-8
DICTIONARY FILE UPDATES: 14 APR 2005 HIGHEST RN 848555-82-8

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

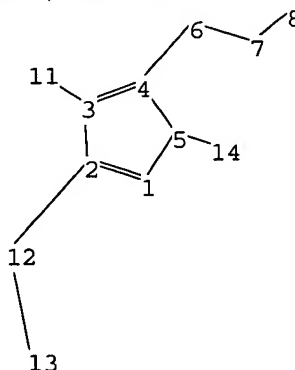
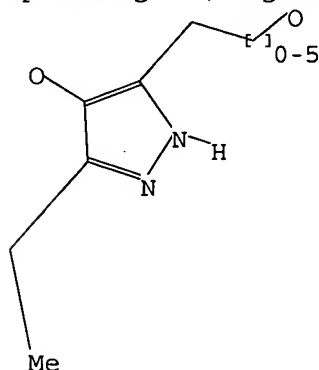
*
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
*

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>

Uploading C:\Program Files\Stnexp\Queries\106570333.str



chain nodes :
6 7 8 11 12 13 14
ring nodes :
1 2 3 4 5
chain bonds :
2-12 3-11 4-6 5-14 6-7 7-8 12-13
ring bonds :
1-2 1-5 2-3 3-4 4-5
exact/norm bonds :
1-2 1-5 2-3 3-4 3-11 4-5 7-8
exact bonds :
2-12 4-6 5-14 6-7 12-13

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 11:CLASS
12:CLASS 13:CLASS 14:CLASS

10/657,033

L15 STRUCTURE UPLOADED

=> s l15

SAMPLE SEARCH INITIATED 19:20:04 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 24 TO ITERATE

100.0% PROCESSED 24 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
 BATCH **COMPLETE**
PROJECTED ITERATIONS: 187 TO 773
PROJECTED ANSWERS: 0 TO 0

L16 0 SEA SSS SAM L15

=> s l15 ful

FULL SEARCH INITIATED 19:20:14 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 645 TO ITERATE

100.0% PROCESSED 645 ITERATIONS 14 ANSWERS
SEARCH TIME: 00.00.01

L17 14 SEA SSS FUL L15

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	161.33	677.86

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-3.65

FILE 'CAPLUS' ENTERED AT 19:20:20 ON 15 APR 2005
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FILE COVERS 1907 - 15 Apr 2005 VOL 142 ISS 17
FILE LAST UPDATED: 14 Apr 2005 (20050414/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

10/657,033

=> s 117

L18 2 L17

=> file reg

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
3.15	681.01

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
0.00	-3.65

CA SUBSCRIBER PRICE

FILE 'REGISTRY' ENTERED AT 19:24:21 ON 15 APR 2005

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STRUCTURE FILE UPDATES: 14 APR 2005 HIGHEST RN 848555-82-8

DICTIONARY FILE UPDATES: 14 APR 2005 HIGHEST RN 848555-82-8

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

Please note that search-term pricing does apply when conducting SmartSELECT searches.

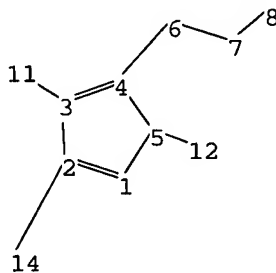
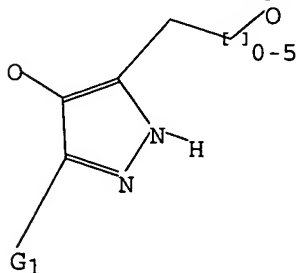
*
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
*

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>

Uploading C:\Program Files\Stnexp\Queries\106570334.str



10/657,033

chain nodes :
6 7 8 11 12 14
ring nodes :
1 2 3 4 5
chain bonds :
2-14 3-11 4-6 5-12 6-7 7-8
ring bonds :
1-2 1-5 2-3 3-4 4-5
exact/norm bonds :
1-2 1-5 2-14 3-11 4-5 7-8
exact bonds :
2-3 3-4 4-6 5-12 6-7
isolated ring systems :
containing 1 :

G1:C,H,O,X,Cb,Ak,CN

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 11:CLASS
12:CLASS 14:CLASS

L19 STRUCTURE UPLOADED

=> s l19
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100.0% PROCESSED 105 ITERATIONS 2 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 1486 TO 2714
PROJECTED ANSWERS: 2 TO 124

L20 2 SEA SSS SAM L19

=> s l19 ful
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FULL SCREEN SEARCH COMPLETED - 2368 TO ITERATE

100.0% PROCESSED 2368 ITERATIONS 63 ANSWERS
SEARCH TIME: 00.00.01

L21 63 SEA SSS FUL L19

=> file caplus		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
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DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-3.65

10/657,033

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FILE COVERS 1907 - 15 Apr 2005 VOL 142 ISS 17
FILE LAST UPDATED: 14 Apr 2005 (20050414/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 121

L22 24 L21

=> d 124 ibib hitstr abs 1-24

L24 NOT FOUND

The L-number entered has not been defined in this session, or it has been deleted. To see the L-numbers currently defined in this session, enter DISPLAY HISTORY at an arrow prompt (=>).

=> d 122 ibib hitstr abs 1-24

L22 ANSWER 1 OF 24 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:308421 CAPLUS

DOCUMENT NUMBER: 140:321351

TITLE: Preparation of pyrazole derivatives as therapeutic agents for HIV mediated diseases

INVENTOR(S): Edwards, Paul John; Jones, Lyn Howard; Mowbray, Charles Eric; Stupple, Paul Anthony; Tran, Isabelle
PATENT ASSIGNEE(S): Pfizer Limited, UK; Pfizer Inc.

SOURCE: PCT Int. Appl., 45 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004031156	A1	20040415	WO 2003-IB4214	20030924
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			

10/657,033

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

US 2005054707 A1 20050310 US 2003-657033 20030905

PRIORITY APPLN. INFO.: GB 2002-23234 A 20021007

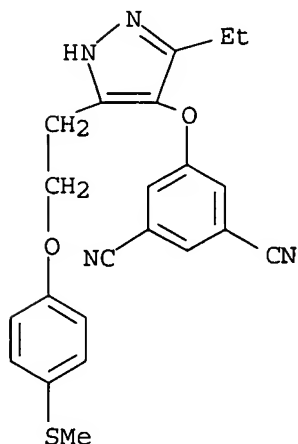
OTHER SOURCE(S): MARPAT 140:321351

IT 678992-80-8P 678992-83-1P 678992-84-2P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of pyrazole derivs. as therapeutic agents for HIV mediated diseases)

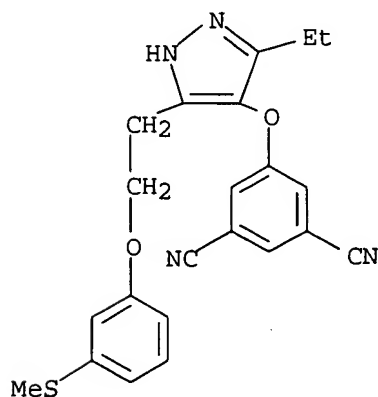
RN 678992-80-8 CAPLUS

CN 1,3-Benzenedicarbonitrile, 5-[[3-ethyl-5-[2-[4-(methylthio)phenoxy]ethyl]-1H-pyrazol-4-yl]oxy] - (9CI) (CA INDEX NAME)



RN 678992-83-1 CAPLUS

CN 1,3-Benzenedicarbonitrile, 5-[[3-ethyl-5-[2-[3-(methylthio)phenoxy]ethyl]-1H-pyrazol-4-yl]oxy] - (9CI) (CA INDEX NAME)

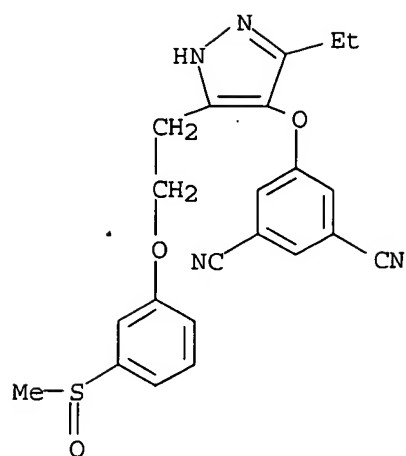


RN 678992-84-2 CAPLUS

CN 1,3-Benzenedicarbonitrile, 5-[[3-ethyl-5-[2-[3-(methylsulfinyl)phenoxy]ethyl]-1H-pyrazol-4-yl]oxy] - (9CI) (CA INDEX NAME)

10/657,033

NAME)



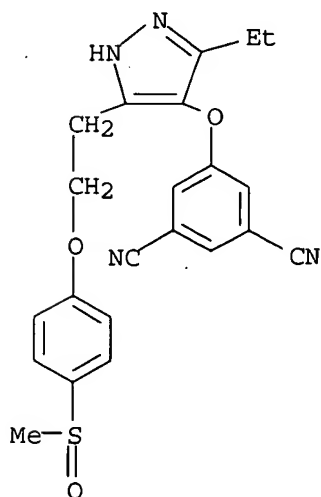
IT 678992-81-9P 678992-82-0P 678992-85-3P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of pyrazole derivs. as therapeutic agents for HIV mediated diseases)

RN 678992-81-9 CAPLUS

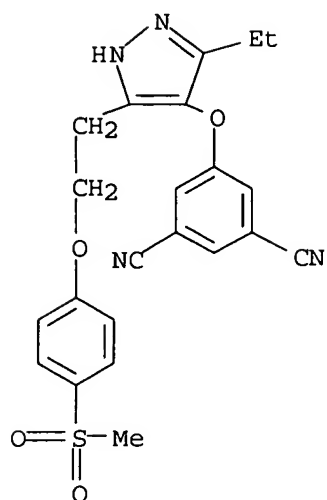
CN 1,3-Benzenedicarbonitrile, 5-[[[3-ethyl-5-[2-[4-(methylsulfinyl)phenoxy]ethyl]-1H-pyrazol-4-yl]oxy]- (9CI) (CA INDEX NAME)



RN 678992-82-0 CAPLUS

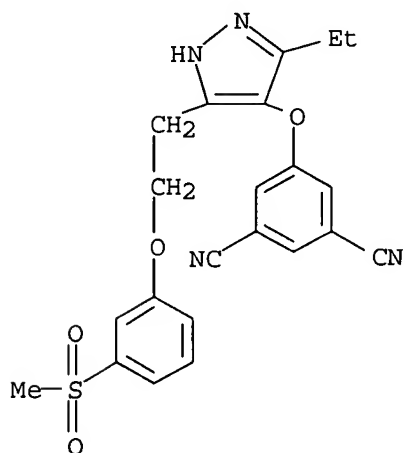
CN 1,3-Benzenedicarbonitrile, 5-[[[3-ethyl-5-[2-[4-(methylsulfonyl)phenoxy]ethyl]-1H-pyrazol-4-yl]oxy]- (9CI) (CA INDEX NAME)

10/657,033



RN 678992-85-3 CAPLUS

CN 1,3-Benzenedicarbonitrile, 5-[[[3-ethyl-5-[2-[3-(methylsulfonyl)phenoxy]ethyl]-1H-pyrazol-4-yl]oxy]- (9CI) (CA INDEX NAME)



IT 473921-46-9P 473921-47-0P

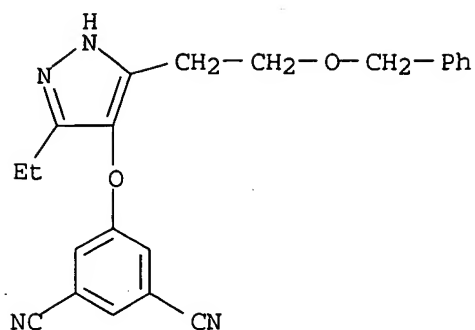
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of pyrazole derivs. as therapeutic agents for HIV mediated diseases)

RN 473921-46-9 CAPLUS

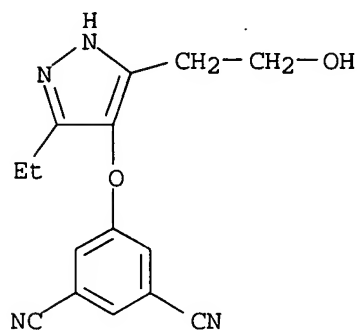
CN 1,3-Benzenedicarbonitrile, 5-[[[3-ethyl-5-[2-(phenylmethoxy)ethyl]-1H-pyrazol-4-yl]oxy]- (9CI) (CA INDEX NAME)

10/657,033

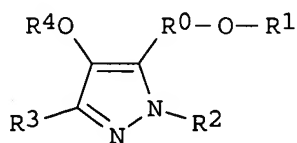


RN 473921-47-0 CAPLUS

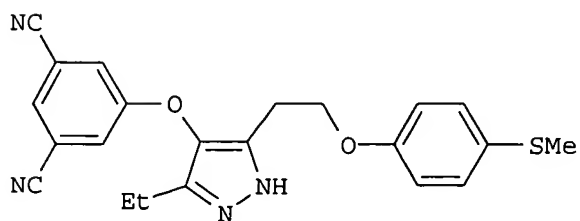
CN 1,3-Benzenedicarbonitrile, 5-[[3-ethyl-5-(2-hydroxyethyl)-1H-pyrazol-4-yl]oxy]- (9CI) (CA INDEX NAME)



GI



I



II

AB The title compds. [I; R0 = absent, alkylene; R1 = Ph substituted by SOyR5, alkylene(SOyR5), SOyCF3, etc.; R2 = H, alkyl, cycloalkyl, etc.; R3 = H, alkyl, cycloalkyl, Ph, etc.; R4 = (un)substituted Ph, naphthyl, pyridyl; R5 = H, alkyl, cycloalkyl, etc.; y = 0-2] which bind to the enzyme reverse transcriptase and are modulators, especially inhibitors thereof, and as such are

useful in the treatment of a variety of disorders including those in which the inhibition' of reverse transcriptase is implicated, were prepared and formulated. Disorders of interest include those caused by Human Immunodeficiency Virus (HIV) and genetically related retroviruses, such as Acquired Immune Deficiency Syndrome (AIDS). Thus, reacting 5-{[3-ethyl-5-(2-hydroxyethyl)-1H-pyrazol-4-yl]oxy}isophthalonitrile (preparation given) with 4-(methylmercapto)phenol afforded I [R0 = (CH2)2; R1 = 4-(MeS)C6H4; R2 = H; R3 = Et; R4 = 3,5-(NC)2C6H3] which showed IC50 of 2 nM against HIV-1 reverse transcriptase. The pharmaceutical composition comprising the compound I is claimed.

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 2 OF 24 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:63587 CAPLUS

DOCUMENT NUMBER: 141:243399

TITLE: Chemistry of Diazopolycarbonyl Compounds: VIII.
Synthesis of Nitrogen-containing Heterocycles via
Transformations of Substituted 2-diazopentane-1,3,5-
triones

AUTHOR(S): Kutkovaya, N. V.; Vyaznikova, N. G.; Zalesov, V. V.

CORPORATE SOURCE: Research Institute of Vaccines and Serum at Federal
State Unitary Enterprise "Biomed", Perm, Russia

SOURCE: Russian Journal of Organic Chemistry (Translation of
Zhurnal Organicheskoi Khimii) (2003), 39(11),
1644-1648

CODEN: RJOCEQ; ISSN: 1070-4280

PUBLISHER: MAIK Nauka/Interperiodica Publishing

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 141:243399

IT 749923-98-6P 749923-99-7P 749924-00-3P

749924-01-4P 749924-02-5P 749924-03-6P

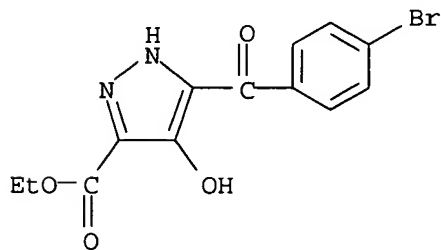
749924-04-7P

RL: SPN (Synthetic preparation); PREP (Preparation)

(synthesis of nitrogen-containing heterocycles via transformations of
substituted diazopentanetriones)

RN 749923-98-6 CAPLUS

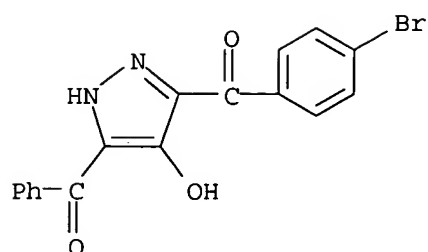
CN 1H-Pyrazole-3-carboxylic acid, 5-(4-bromobenzoyl)-4-hydroxy-, ethyl ester
(9CI) (CA INDEX NAME)



RN 749923-99-7 CAPLUS

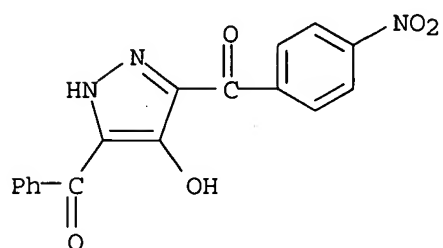
CN Methanone, (5-benzoyl-4-hydroxy-1H-pyrazol-3-yl)(4-bromophenyl)- (9CI)
(CA INDEX NAME)

10/657,033



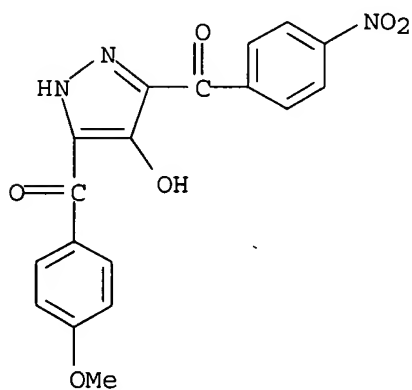
RN 749924-00-3 CAPLUS

CN Methanone, (5-benzoyl-4-hydroxy-1H-pyrazol-3-yl) (4-nitrophenyl) - (9CI)
(CA INDEX NAME)



RN 749924-01-4 CAPLUS

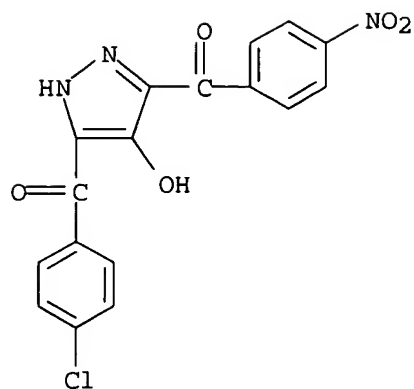
CN Methanone, [4-hydroxy-5-(4-methoxybenzoyl)-1H-pyrazol-3-yl] (4-nitrophenyl) -
(9CI) (CA INDEX NAME)



RN 749924-02-5 CAPLUS

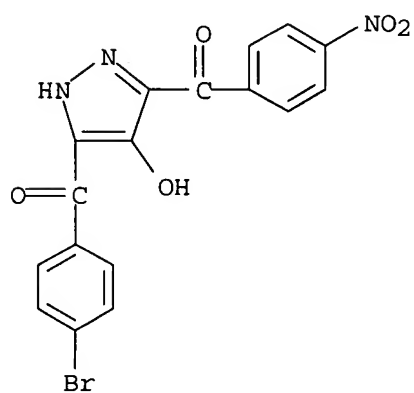
CN Methanone, [5-(4-chlorobenzoyl)-4-hydroxy-1H-pyrazol-3-yl] (4-nitrophenyl) -
(9CI) (CA INDEX NAME)

10/657,033



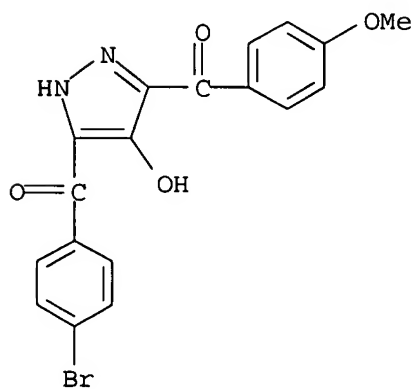
RN 749924-03-6 CAPLUS

CN Methanone, [5-(4-bromobenzoyl)-4-hydroxy-1H-pyrazol-3-yl] (4-nitrophenyl) -
(9CI) (CA INDEX NAME)



RN 749924-04-7 CAPLUS

CN Methanone, [5-(4-bromobenzoyl)-4-hydroxy-1H-pyrazol-3-yl] (4-methoxyphenyl) -
(9CI) (CA INDEX NAME)



AB Et 5-aryl-2-diazo-3,5-dioxopentanoates and 1,5-diaryl-2-diazopentane-1,3,5-triones are partially enolized in solns. By O-methylation of enol forms of diazo esters with diazomethane Et 5-aryl-2-diazo-5-methoxy-3-oxopent-4-enoates were prepared. Concurrently with the O-methylation the diazo esters undergo heterocyclization into 3,5-disubstituted 4-hydroxypyrazoles which under the reaction condition suffer O- and N-methylation by excess diazomethane. 3,5-Diaroyl-4-hydroxypyrazoles were also obtained from diazopentane-triones but here triethylamine served as the cyclization reagent.

REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 4 OF 24 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2002:832763 CAPLUS

DOCUMENT NUMBER: 137:337884

TITLE: Preparation of aryloxy pyrazole derivatives as reverse transcriptase inhibitors for treating HIV

INVENTOR(S): Jones, Lyn Howard; Mowbray, Charles Eric; Price, Davis Anthony; Selby, Matthew Duncan; Stupple, Paul Anthony

PATENT ASSIGNEE(S): Pfizer Limited, UK; Pfizer Inc.

SOURCE: PCT Int. Appl., 306 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002085860	A1	20021031	WO 2002-IB1234	20020404
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
CA 2443449	AA	20021031	CA 2002-2443449	20020404
EP 1377556	A1	20040107	EP 2002-708600	20020404
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR			
EE 200300497	A	20040216	EE 2003-497	20020404
BR 2002008811	A	20040309	BR 2002-8811	20020404
JP 2004531535	T2	20041014	JP 2002-583387	20020404
US 2003100554	A1	20030529	US 2002-118512	20020405
ZA 2003007095	A	20040910	ZA 2003-7095	20030910
NO 2003004523	A	20031209	NO 2003-4523	20031009
PRIORITY APPLN. INFO.:			GB 2001-8999	A 20010410
			GB 2001-27426	A 20011115
			US 2001-289570P	P 20010508
			US 2002-346727P	P 20020107
			WO 2002-IB1234	W 20020404

OTHER SOURCE(S): MARPAT 137:337884

IT 473921-40-3P, 3-[5-[2-(Benzyloxy)ethyl]-3-ethyl-1H-pyrazol-4-

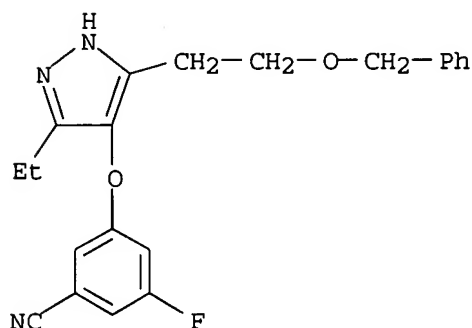
yl]oxy]-5-fluorobenzonitrile **473921-41-4P**, 3-[[3-Ethyl-5-(2-hydroxyethyl)-1H-pyrazol-4-yl]oxy]-5-fluorobenzonitrile **473921-46-9P**, 5-[[5-[2-(Benzyloxy)ethyl]-3-ethyl-1H-pyrazol-4-yl]oxy]isophthalonitrile

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(drug candidate; preparation of aryloxy pyrazole derivs. as reverse transcriptase inhibitors for treating HIV)

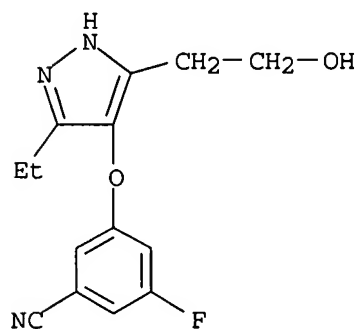
RN 473921-40-3 CAPLUS

CN Benzonitrile, 3-[[3-ethyl-5-[2-(phenylmethoxy)ethyl]-1H-pyrazol-4-yl]oxy]-5-fluoro- (9CI) (CA INDEX NAME)



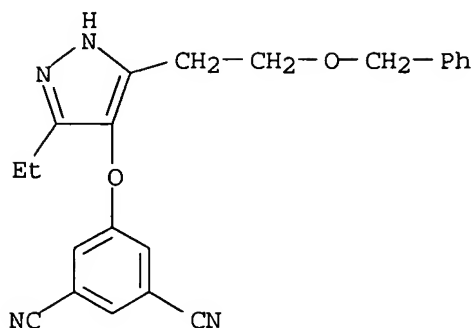
RN 473921-41-4 CAPLUS

CN Benzonitrile, 3-[[3-ethyl-5-(2-hydroxyethyl)-1H-pyrazol-4-yl]oxy]-5-fluoro- (9CI) (CA INDEX NAME)



RN 473921-46-9 CAPLUS

CN 1,3-Benzenedicarbonitrile, 5-[[3-ethyl-5-[2-(phenylmethoxy)ethyl]-1H-pyrazol-4-yl]oxy]- (9CI) (CA INDEX NAME)



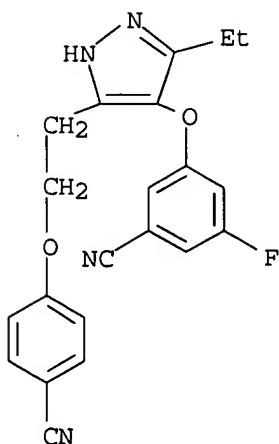
IT 473921-42-5P, 3-[[5-[2-(4-Cyanophenoxy)ethyl]-3-ethyl-1H-pyrazol-4-yl]oxy]-5-fluorobenzonitrile 473921-43-6P, 3-Fluoro-5-[[3-ethyl-5-(2-((2-methyl-3-pyridyl)oxy)ethyl)-1H-pyrazol-4-yl]oxy]benzonitrile 473921-44-7P, 3-Fluoro-5-[[3-ethyl-5-(2-((3-pyridyl)oxy)ethyl)-1H-pyrazol-4-yl]oxy]benzonitrile 473921-45-8P, 3-Fluoro-5-[[3-ethyl-5-(2-((2-amino-3-pyridyl)oxy)ethyl)-1H-pyrazol-4-yl]oxy]benzonitrile 473921-47-0P, 5-[[3-Ethyl-5-(2-hydroxyethyl)-1H-pyrazol-4-yl]oxy]isophthalonitrile

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of aryloxy pyrazole derivs. as reverse transcriptase inhibitors for treating HIV)

RN 473921-42-5 CAPLUS

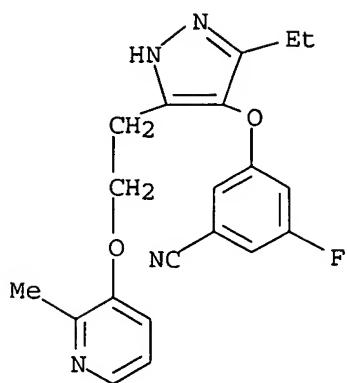
CN Benzonitrile, 3-[[5-[2-(4-cyanophenoxy)ethyl]-3-ethyl-1H-pyrazol-4-yl]oxy]-5-fluoro- (9CI) (CA INDEX NAME)



RN 473921-43-6 CAPLUS

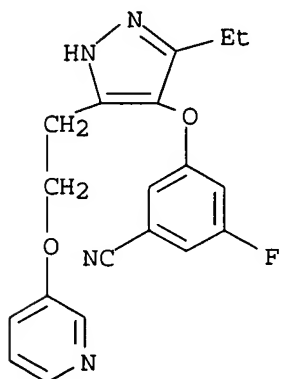
CN Benzonitrile, 3-[[3-ethyl-5-[2-[[2-(4-cyanophenoxy)ethyl]-1H-pyrazol-4-yl]oxy]ethyl]-1H-pyrazol-4-yl]oxy]-5-fluoro- (9CI) (CA INDEX NAME)

10/657,033



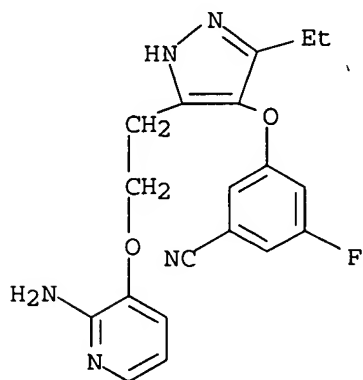
RN 473921-44-7 CAPLUS

CN Benzonitrile, 3-[[3-ethyl-5-[2-(3-pyridinyloxy)ethyl]-1H-pyrazol-4-yl]oxy]-5-fluoro- (9CI) (CA INDEX NAME)



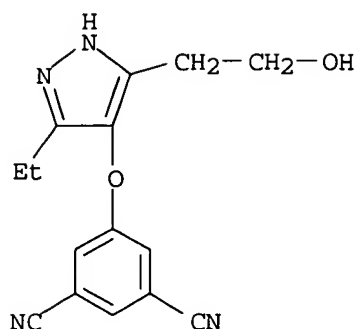
RN 473921-45-8 CAPLUS

CN Benzonitrile, 3-[[5-[2-[(2-amino-3-pyridinyl)oxy]ethyl]-3-ethyl-1H-pyrazol-4-yl]oxy]-5-fluoro- (9CI) (CA INDEX NAME)

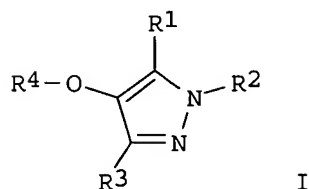


RN 473921-47-0 CAPLUS

CN 1,3-Benzenedicarbonitrile, 5-[[3-ethyl-5-(2-hydroxyethyl)-1H-pyrazol-4-yl]oxy]- (9CI) (CA INDEX NAME)



GI



I

AB This invention relates to pyrazole derivs. (shown as I; e.g. 2-Amino-6-[[4-(3,5-dichlorophenoxy)-3,5-diethyl-1H-pyrazol-1-yl]methyl]-4(3H)-pyrimidinone) or pharmaceutically acceptable salts, solvates or derivative thereof, wherein R₁ to R₄ are defined below, and to processes for the preparation thereof, intermediates used in their preparation of, compns. containing

them and the uses of such derivs. The compds. of the present invention bind to the enzyme reverse transcriptase and are modulators, especially inhibitors thereof. As such the compds. of the present invention are useful in the treatment of a variety of disorders including those in which the inhibition of reverse transcriptase is implicated. Disorders of interest include those caused by Human Immunodeficiency Virus (HIV) and genetically related retroviruses, such as Acquired Immune Deficiency Syndrome (AIDS). In tests of inhibition of HIV-1 reverse transcriptase enzyme, the claimed compds. 2-amino-6-[[4-(3,5-dichlorophenoxy)-3,5-diethyl-1H-pyrazol-1-yl]methyl]-4(3H)-pyrimidinone, 3,5-dimethyl-4-[[3,5-diethyl-1-(2-hydroxyethyl)-1H-pyrazol-4-yl]oxy]benzonitrile and 1-(3-azetidiny)-4-(3,5-dichlorophenoxy)-3,5-diethyl-1H-pyrazole had IC₅₀ values of 39,000, 3,200 and 248 nM, resp. In I: R₁ is H, C₁-C₆ alkyl, C₃-C₇ cycloalkyl, Ph, benzyl, halo, -CN, -OR₇, -CO₂R₁₀, -CONR₅R₁₀, R₈ or R₉. R₂ is H, C₁-C₆ alkyl, C₃-C₆ alkenyl, C₃-C₆ alkynyl, C₃-C₇ cycloalkyl, C₃-C₇ cycloalkenyl, Ph, benzyl, R₈ or R₉; or, R₁ and R₂, when taken together, represent unbranched C₃-C₄ alkylene. R₃ is H, C₁-C₆ alkyl, C₃-C₇ cycloalkyl, Ph, benzyl, halo, -CN, -OR₇, -CO₂R₅, -CONR₅R₅, R₈ or R₉; R₄ is Ph, naphthyl or pyridyl. Definitions of R₅ and R₇-R₁₀ and addnl. specifications are given in the claims. Included are 283 claimed-compound preps. and 115 intermediate preps.

REFERENCE COUNT:

8

THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

10/657,033

L22 ANSWER 8 OF 24 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1999:375284 CAPLUS
DOCUMENT NUMBER: 131:31936
TITLE: Selective β 3 adrenergic agonists
INVENTOR(S): Crowell, Thomas Alan; Jones, Charles David; Shuker, Anthony John
PATENT ASSIGNEE(S): Eli Lilly and Company, USA
SOURCE: Eur. Pat. Appl., 48 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 921120	A1	19990609	EP 1998-309868	19981202
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
ZA 9811026	A	20000602	ZA 1998-11026	19981202
CA 2312987	AA	19990617	CA 1998-2312987	19981204
WO 9929673	A1	19990617	WO 1998-US25831	19981204
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
AU 9916281	A1	19990628	AU 1999-16281	19981204
US 6046227	A	20000404	US 1998-206107	19981204
JP 2001525399	T2	20011211	JP 2000-524270	19981204
US 6617347	B1	20030909	US 1999-443272	19991118
PRIORITY APPLN. INFO.:				US 1997-67599P P 19971205
				US 1998-204372 A1 19981202
				US 1998-206107 A3 19981204
				WO 1998-US25831 W 19981204

OTHER SOURCE(S): MARPAT 131:31936

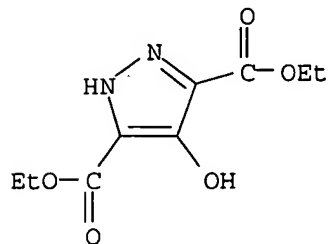
IT 23705-86-4P 226989-47-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(pyrazole derivs. as selective β 3 adrenergic agonists)

RN 23705-86-4 CAPLUS

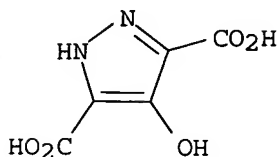
CN 1H-Pyrazole-3,5-dicarboxylic acid, 4-hydroxy-, diethyl ester (9CI) (CA INDEX NAME)



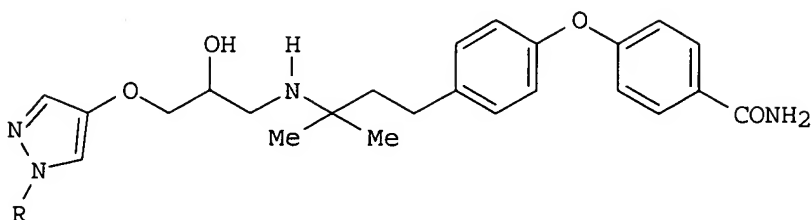
10/657,033

RN 226989-47-5 CAPLUS

CN 1H-Pyrazole-3,5-dicarboxylic acid, 4-hydroxy- (9CI) (CA INDEX NAME)



GI



I

AB Pyrazole derivs. such as I (R = H) were prepared as β_3 adrenergic agonists. Thus, 1.75 g (S)-1-benzyl-4-glycidylpyrazole and 3.6 g 4-Me₂C(NH₂)CH₂CH₂C₆H₄OC₆H₄CONH₂-4 were heated to 45° for 72 h in 100 mL EtOH to give I (R = benzyl) in 52.5% yield. Hydrogenolysis of I (benzyl) over 20% Pd(OH)₂/C in EtOH at 40° for 72 h gave I (R = H) in 32% yield. A combinatorial chemical example was also given. In evaluating β_3 agonist activity (cAMP assays), the present compds. showed at least 30%, preferably 50%, and most preferably >85% of isoproterenol's response at a single dose of 50 mmol.

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 9 OF 24 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1999:162019 CAPLUS

DOCUMENT NUMBER: 130:237515

TITLE: Selective dopamine receptors: synthesis, complexing properties, and molecular modeling studies of new podands derived from 4-hydroxy-1H-pyrazole

AUTHOR(S): Rodriguez-Franco, Maria Isabel; San Lorenzo, Patricia; Martinez, Ana; Navarro, Pilar

CORPORATE SOURCE: Instituto de Quimica Medica (C.S.I.C.), Madrid, 28006, Spain

SOURCE: Tetrahedron (1999), 55(9), 2763-2772

CODEN: TETRAB; ISSN: 0040-4020

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 130:237515

IT 23705-86-4

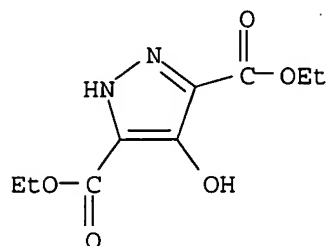
RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of hydroxypyrazole podands, mol. modeling, and complexation behavior toward cations and dopamine and norepinephrine)

RN 23705-86-4 CAPLUS

10/657,033

CN 1H-Pyrazole-3,5-dicarboxylic acid, 4-hydroxy-, diethyl ester (9CI) (CA INDEX NAME)



IT 221347-44-0P 221347-45-1P

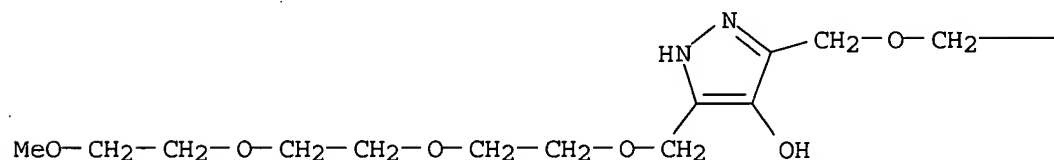
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of hydroxypyrazole podands, mol. modeling, and complexation behavior toward cations and dopamine and norepinephrine)

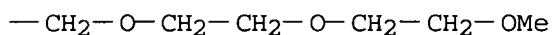
RN 221347-44-0 CAPLUS

CN 1H-Pyrazol-4-ol, 3,5-bis(2,5,8,11-tetraoxadodec-1-yl)- (9CI) (CA INDEX NAME)

PAGE 1-A



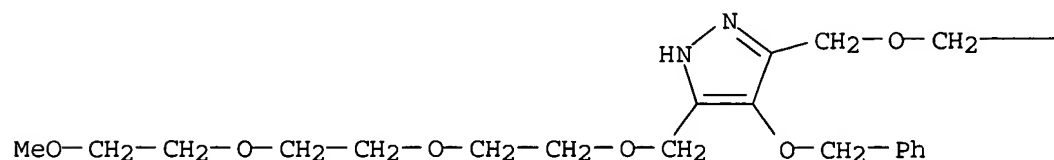
PAGE 1-B



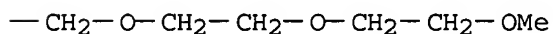
RN 221347-45-1 CAPLUS

CN 1H-Pyrazole, 4-(phenylmethoxy)-3,5-bis(2,5,8,11-tetraoxadodec-1-yl)- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



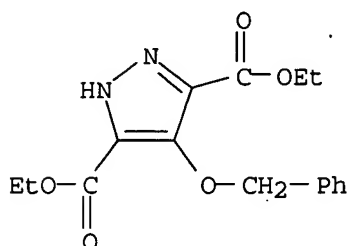
10/657,033

IT 221347-37-1P

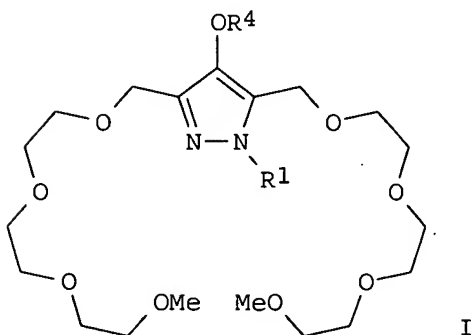
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of hydroxypyrazole podands, mol. modeling, and complexation
behavior toward cations and dopamine and norepinephrine)

RN 221347-37-1 CAPLUS

CN 1H-Pyrazole-3,5-dicarboxylic acid, 4-(phenylmethoxy)-, diethyl ester (9CI)
(CA INDEX NAME)



GI



AB New podands, I (R1 = R4 = CH2Ph, H; R1 = CH2Ph, R4 = H; R1 = H, R4 = CH2Ph), derived from 4-hydroxy-1H-pyrazole have been prepared. Their complexing properties toward cations (Na⁺, K⁺, NH₄⁺) and some neurotransmitters (dopamine and norepinephrine) have been studied, using biphasic extraction expts., mol. modeling, and a NMR titration. Podand I (R1 = CH2Ph, R4 = H), 1-benzyl-4-hydroxy-3,5-bis(2,5,8,11-tetraoxadodecan-1-yl)-1H-pyrazole, showed an interesting selective complexation of dopamine.

REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 10 OF 24 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1996:162161 CAPLUS

DOCUMENT NUMBER: 124:317104

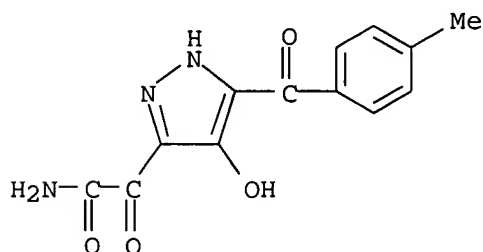
TITLE: Chemistry of diazopolycarbonyl compounds. II.
Synthesis of aroylacetyl derivatives of diazopyruvic
acid esters and their reaction with ammonia and
o-phenylenediamine

AUTHOR(S): Zalesov, V. V.; Vyaznikova, N. G.; Andreichikov, Yu.
S.

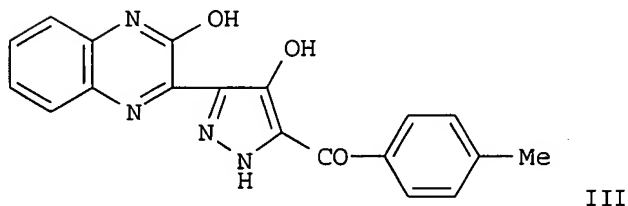
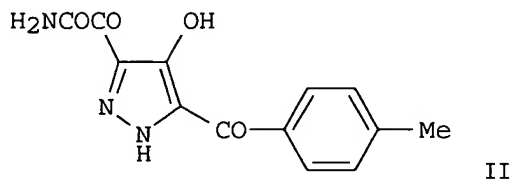
CORPORATE SOURCE: Perm. Farm. Inst., Russia

10/657,033

SOURCE: Zhurnal Organicheskoi Khimii (1995), 31(8), 1213-17
CODEN: ZORKAE; ISSN: 0514-7492
PUBLISHER: Nauka
DOCUMENT TYPE: Journal
LANGUAGE: Russian
IT 176375-05-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 176375-05-6 CAPLUS
CN 1H-Pyrazole-3-acetamide, 4-hydroxy-5-(4-methylbenzoyl)- α -oxo- (9CI)
(CA INDEX NAME)



GI

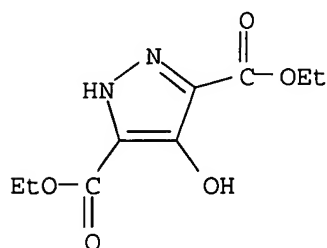


AB (Z)-R1OCOCOC(:N2)COCH:C(OH)C6H4R2-4 (I; R1 = Et, Pr, Bu; R2 = H, Me, OMe, Cl, Br) were prepared by reaction of 5-aryl-2,3-furandiones with R1OCOCOCHN2. Reaction of I with NH4OH gave pyrazoles, e.g., II, and reaction with o-phenylenediamine gave pyrazolylquinoxalines, e.g., III. Other quinoxalines were prepared from the arylfurandiones and o-phenylenediamine.

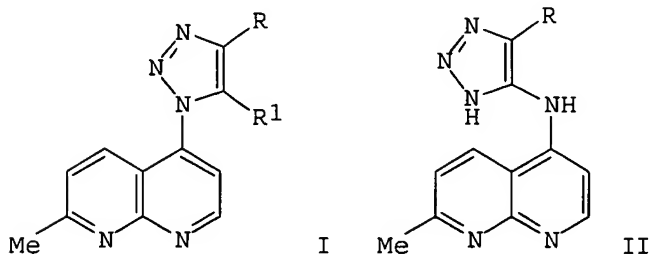
L22 ANSWER 21 OF 24 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1977:89704 CAPLUS
DOCUMENT NUMBER: 86:89704
TITLE: Synthesis and biological activity of
1,2,3-triazolo-1,8-naphthyridine derivatives

10/657,033

AUTHOR(S): Livi, O.; Ferrarini, P. L.; Tonetti, I.
CORPORATE SOURCE: Ist. Chim. Farm., Univ. Pisa, Pisa, Italy
SOURCE: Farmaco, Edizione Scientifica (1976), 31(11), 797-808
CODEN: FRPSAX; ISSN: 0430-0920
DOCUMENT TYPE: Journal
LANGUAGE: Italian
OTHER SOURCE(S): CASREACT 86:89704
IT 23705-86-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 23705-86-4 CAPLUS
CN 1H-Pyrazole-3,5-dicarboxylic acid, 4-hydroxy-, diethyl ester (9CI) (CA
INDEX NAME)



GI



AB Triazolylnaphthyridines I (R = Ph, CO₂Et, cyano, R₁ = NH₂; R = CO₂Et, CO₂H, R₁ = Me, Ph, 4-O₂NC₆H₄; R = Ac, Bz, R₁ = Me, Ph; R = Ph, CONHPh, R₁ = Me; R = CO₂Et, R₁ = CH₂CO₂Et; R = H, R₁ = 4-O₂NC₆H₄) were prepared by reaction of 2-methyl-5-azido-1,8-naphthyridine with RCH₂CN or RCOCH₂R₁. I (R₁ = NH₂) rearranged on heating to the triazolyaminonaphthyridines II. I (R = CONHPh, R₁ = Me) had twice the analgesic activity of phenylbutazone. I (R = Ac, Ph, R₁ = Me) and II (R = Ph) had sedative activity (no data) and II (R = Ph, CO₂H) were fungicidal.

L22 ANSWER 22 OF 24 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1977:43964 CAPLUS

DOCUMENT NUMBER: 86:43964

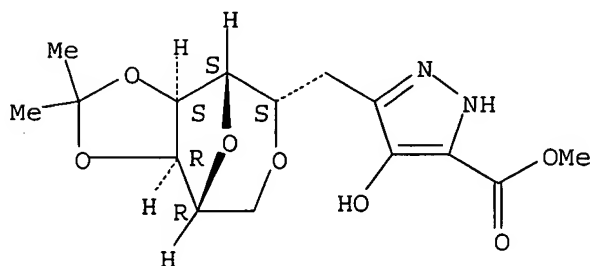
TITLE: Syntheses of C-nucleosides. IX. Reactions of D,L-3,4-di-O-isopropylidene-2,5-anhydroallose with Wittig reagents. Syntheses of bis-homo anhydro-C-nucleosides

AUTHOR(S): Just, George; Ramjeesingh, Mohabir; Liak, Teng Jiam
CORPORATE SOURCE: Dep. Chem., McGill Univ., Montreal, QC, Can.

10/657,033

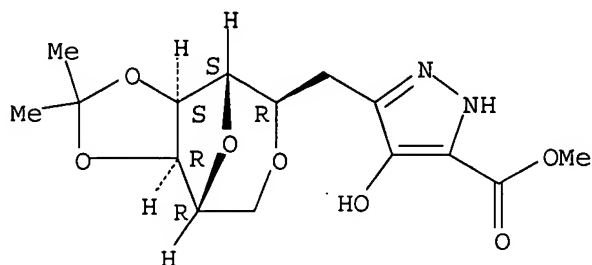
SOURCE: Canadian Journal of Chemistry (1976), 54(18), 2940-7
CODEN: CJCHAG; ISSN: 0008-4042
DOCUMENT TYPE: Journal
LANGUAGE: English
IT 61407-36-1P 61407-37-2P 61407-38-3P
61407-39-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 61407-36-1 CAPLUS
CN D-glycero-D-allo-Heptitol, 2,7:3,6-dianhydro-1-deoxy-1-[4-hydroxy-5-(methoxycarbonyl)-1H-pyrazol-3-yl]-4,5-O-(1-methylethylidene)-, rel- (9CI)
(CA INDEX NAME)

Relative stereochemistry.



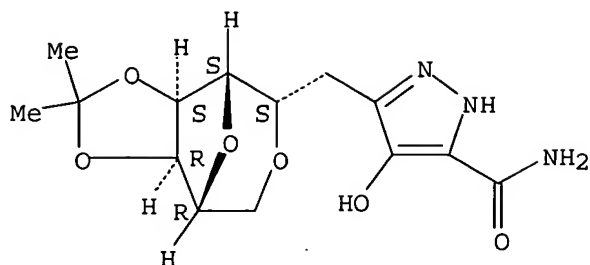
RN 61407-37-2 CAPLUS
CN D-glycero-D-altro-Heptitol, 2,7:3,6-dianhydro-1-deoxy-1-[4-hydroxy-5-(methoxycarbonyl)-1H-pyrazol-3-yl]-4,5-O-(1-methylethylidene)-, rel- (9CI)
(CA INDEX NAME)

Relative stereochemistry.



RN 61407-38-3 CAPLUS
CN D-glycero-D-allo-Heptitol, 1-[5-(aminocarbonyl)-4-hydroxy-1H-pyrazol-3-yl]-2,7:3,6-dianhydro-1-deoxy-4,5-O-(1-methylethylidene)-, rel- (9CI) (CA INDEX NAME)

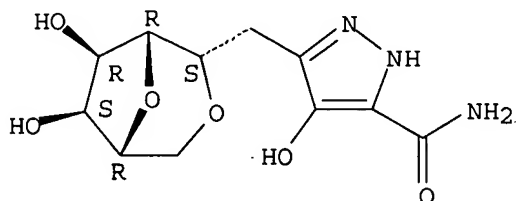
Relative stereochemistry.



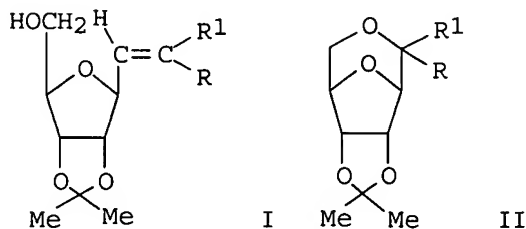
RN 61407-39-4 CAPLUS

CN D-glycero-D-allo-Heptitol, 1-[5-(aminocarbonyl)-4-hydroxy-1H-pyrazol-3-yl]-2,7:3,6-dianhydro-1-deoxy-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



GI



AB The NMR spectra of the two anomers of 1-O-acetyl-3,4-di-O-isopropylidene-2,5-anhydro-D,L-allose are discussed. Wittig reactions of D,L-3,4-di-O-isopropylidene-2,5-anhydroallose gave the olefins I (R = H, R1 = CO2Et; R = Br, R1 = CO2Et; R = CO2Et, R1 = Br; R = H, R1 = COCO2Et) and an internal Michael addition product II (R = H, R1 = CH2COCO2Et; R = CH2COCO2Et, R1 = H). II gave two bis-homo anhydro-C-nucleosides having 6-azauracil and 4-hydroxy-5-carboxamidopyrazole base.

L22 ANSWER 23 OF 24 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1970:445752 CAPLUS

DOCUMENT NUMBER: 73:45752

TITLE: Hydrazine reactions. XII. Reaction of 4-ulose hydrazones to 4-hydroxypyridazines and of 3-ulose hydrazones to 4-hydroxypyrazoles

AUTHOR(S): Paulsen, Hans; Steinert, Karin; Steinert, Gerd
CORPORATE SOURCE: Inst. Org. Chem., Univ. Hamburg, Hamburg, Fed. Rep. Ger.

SOURCE: Chemische Berichte (1970), 103(6), 1846-54

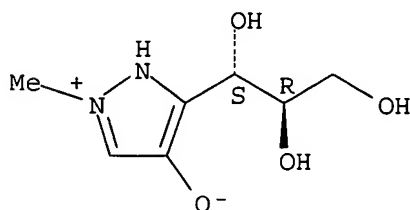
CODEN: CHBEAM; ISSN: 0009-2940

DOCUMENT TYPE: Journal
 LANGUAGE: German
 OTHER SOURCE(S): CASREACT 73:45752
 IT 29673-22-1P 29906-02-3P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 29673-22-1 CAPLUS

CN Pyrazolium, 4-hydroxy-2-methyl-5-(D-erythro-1,2,3-trihydroxypropyl)-,
 hydroxide, inner salt (8CI) (CA INDEX NAME)

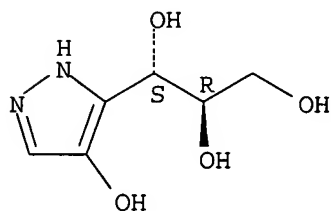
Absolute stereochemistry.



RN 29906-02-3 CAPLUS

CN 1,2,3-Propanetriol, 1-(4-hydroxypyrazol-3-yl)-, D-erythro- (8CI) (CA
 INDEX NAME)

Absolute stereochemistry.



GI For diagram(s), see printed CA Issue.

AB 2,3:5,6-Di-O-isopropylidene-D-xylo-hexos-4-ulose hydrazone di-Me acetal
 was cyclized with 2N HCl to give (via the corresponding 1:1 4- and
 5-hydroxypyridazinium chloride, with subsequent HCl cleavage)
 3-(D-glycero-1,2-dihydroxyethyl)-4(1H)- and -5(2H)-pyridazinone (I and
 II). The corresponding N'-methylhydrazone gave only the 5-hydroxy derivative,
 isolated as a zwitterion. 3,5-Dideoxy-3-hydrazino-1,2-O-isopropylidene-D-
 ribofuranose p-toluenesulfonate, prepared from 5-deoxy-1,2-O-isopropylidene-
 3-O-p-tolylsulfonyl-D-xylofuranose and H₂NNH₂, gave with 2N HCl
 5-(D-glycero-1-hydroxyethyl)pyrazole (III, R = Me). Similarly,
 1,2:5,6-Di-O-isopropylidene-α-D-ribo-hexofuranos-3-ulose hydrazone
 gave 4-hydroxy-5-(D-erythro-1,2,3-trihydroxypropyl)pyrazole [III, R =
 CH(OH)CH₂OH]. NMR and uv data were reported.

L22 ANSWER 24 OF 24 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1969:47359 CAPLUS

DOCUMENT NUMBER: 70:47359

TITLE: Esters of 4-hydroxypyrazole-3,5-dicarboxylic acid

AUTHOR(S): Begtrup, Mikael; Larsen, P. Skov; Pedersen, Christian

CORPORATE SOURCE: Org.-Kem. Lab., Polytek. Laereanstalt, Lyngby, Den.

SOURCE: Acta Chemica Scandinavica (1947-1973) (1968), 22(8),
 2476-8

10/657,033

CODEN: ACSAA4; ISSN: 0001-5393

DOCUMENT TYPE:

Journal

LANGUAGE:

English

OTHER SOURCE(S):

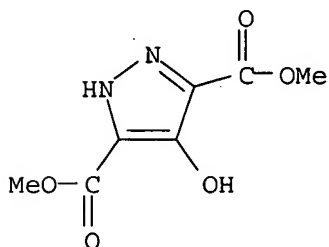
CASREACT 70:47359

IT 23705-85-3P 23705-86-4P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

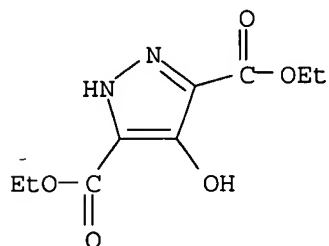
RN 23705-85-3 CAPLUS

CN 1H-Pyrazole-3,5-dicarboxylic acid, 4-hydroxy-, dimethyl ester (9CI) (CA
INDEX NAME)



RN 23705-86-4 CAPLUS

CN 1H-Pyrazole-3,5-dicarboxylic acid, 4-hydroxy-, diethyl ester (9CI) (CA
INDEX NAME)



AB The base catalyzed reaction of di-Me diazomalonate with di-Me malonate (I) gives a high yield of di-Me 4-hydroxypyrazole-3,5-dicarboxylate (II). The corresponding di-Et ester was obtained in low yield only. The mechanism of the formation of II as a by-product in the reaction of PhN3 with I is discussed.

=> log y

COST IN U.S. DOLLARS

SINCE FILE

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FULL ESTIMATED COST

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961.80

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

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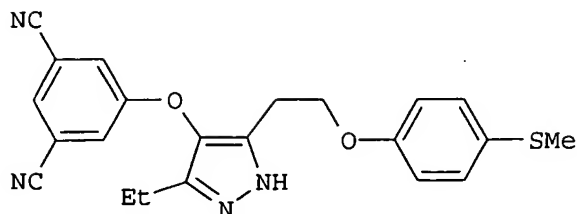
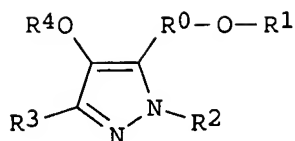
SESSION

CA SUBSCRIBER PRICE

-17.52

-21.17

STN INTERNATIONAL LOGOFF AT 19:26:04 ON 15 APR 2005



AB The title compds. [I; R0 = absent, alkylene; R1 = Ph substituted by SOyR5, alkylene(SOyR5), SOyCF3, etc.; R2 = H, alkyl, cycloalkyl, etc.; R3 = H, alkyl, cycloalkyl, Ph, etc.; R4 = (un)substituted Ph, naphthyl, pyridyl; R5 = H, alkyl, cycloalkyl, etc.; y = 0-2] which bind to the enzyme reverse transcriptase and are modulators, especially inhibitors thereof, and as such are useful in the treatment of a variety of disorders including those in which the inhibition of reverse transcriptase is implicated, were prepared and formulated. Disorders of interest include those caused by Human Immunodeficiency Virus (HIV) and genetically related retroviruses, such as Acquired Immune Deficiency Syndrome (AIDS). Thus, reacting 5-([3-ethyl-5-(2-hydroxyethyl)-1H-pyrazol-4-yl]oxy)isophthalonitrile (preparation given) with 4-(methylmercapto)phenol afforded I [R0 = (CH2)2; R1 = 4-(MeS)C6H4; R2 = H; R3 = Et; R4 = 3,5-(NC)2C6H3] which showed IC50 of 2 nM against HIV-1 reverse transcriptase. The pharmaceutical composition comprising the compound I is claimed.

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d l14 ibib hitstr abs 2

L14 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2002:832763 CAPLUS

DOCUMENT NUMBER: 137:337884

TITLE: Preparation of aryloxy pyrazole derivatives as reverse transcriptase inhibitors for treating HIV

INVENTOR(S): Jones, Lyn Howard; Mowbray, Charles Eric; Price, Davis Anthony; Selby, Matthew Duncan; Stupple, Paul Anthony

PATENT ASSIGNEE(S): Pfizer Limited, UK; Pfizer Inc.

SOURCE: PCT Int. Appl., 306 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002085860	A1	20021031	WO 2002-IB1234	20020404
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,				

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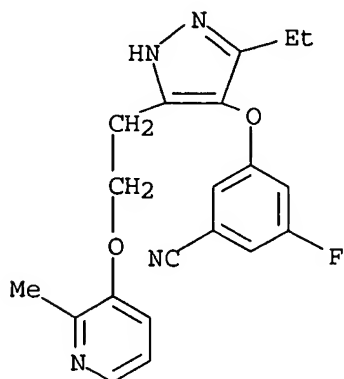
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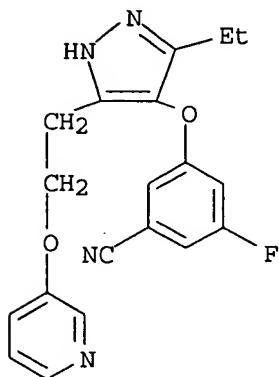
10/657,033

CN Benzonitrile, 3-[[3-ethyl-5-[2-[(2-methyl-3-pyridinyl)oxy]ethyl]-1H-pyrazol-4-yl]oxy]-5-fluoro- (9CI) (CA INDEX NAME)



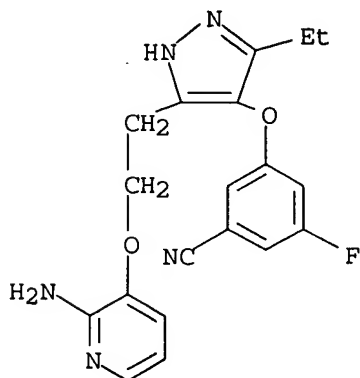
RN 473921-44-7 CAPLUS

CN Benzonitrile, 3-[[3-ethyl-5-[2-(3-pyridinyloxy)ethyl]-1H-pyrazol-4-yl]oxy]-5-fluoro- (9CI) (CA INDEX NAME)

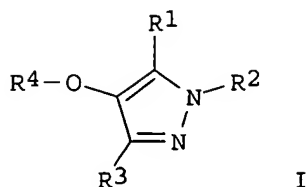


RN 473921-45-8 CAPLUS

CN Benzonitrile, 3-[[5-[2-[(2-amino-3-pyridinyl)oxy]ethyl]-3-ethyl-1H-pyrazol-4-yl]oxy]-5-fluoro- (9CI) (CA INDEX NAME)



GI



AB This invention relates to pyrazole derivs. (shown as I; e.g. 2-Amino-6-[[4-(3,5-dichlorophenoxy)-3,5-diethyl-1H-pyrazol-1-yl]methyl]-4(3H)-pyrimidinone) or pharmaceutically acceptable salts, solvates or derivative thereof, wherein R1 to R4 are defined below, and to processes for the preparation thereof, intermediates used in their preparation of, compns. containing

them and the uses of such derivs. The compds. of the present invention bind to the enzyme reverse transcriptase and are modulators, especially inhibitors thereof. As such the compds. of the present invention are useful in the treatment of a variety of disorders including those in which the inhibition of reverse transcriptase is implicated. Disorders of interest include those caused by Human Immunodeficiency Virus (HIV) and genetically related retroviruses, such as Acquired Immune Deficiency Syndrome (AIDS). In tests of inhibition of HIV-1 reverse transcriptase enzyme, the claimed compds. 2-amino-6-[[4-(3,5-dichlorophenoxy)-3,5-diethyl-1H-pyrazol-1-yl]methyl]-4(3H)-pyrimidinone, 3,5-dimethyl-4-[[3,5-diethyl-1-(2-hydroxyethyl)-1H-pyrazol-4-yl]oxy]benzonitrile and 1-(3-azetidiny)-4-(3,5-dichlorophenoxy)-3,5-diethyl-1H-pyrazole had IC50 values of 39,000, 3,200 and 248 nM, resp. In I: R1 is H, C1-C6 alkyl, C3-C7 cycloalkyl, Ph, benzyl, halo, -CN, -OR7, -CO2R10, -CONR5R10, R8 or R9. R2 is H, C1-C6 alkyl, C3-C6 alkenyl, C3-C6 alkynyl, C3-C7 cycloalkyl, C3-C7 cycloalkenyl, Ph, benzyl, R8 or R9; or, R1 and R2, when taken together, represent unbranched C3-C4 alkylene. R3 is H, C1-C6 alkyl, C3-C7 cycloalkyl, Ph, benzyl, halo, -CN, -OR7, -CO2R5, -CONR5R5, R8 or R9; R4 is Ph, naphthyl or pyridyl. Definitions of R5 and R7-R10 and addnl. specifications are given in the claims. Included are 283 claimed-compound preps. and 115 intermediate preps.

REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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COST IN U.S. DOLLARS

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ENTRY	SESSION
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FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
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